Helping Students Learn Quantum Mechanics using Research-Validated Learning Tools

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The development and implementation of research-validated instructional tools has shown promise in improving student learning in not only introductory physics courses, but also upper level quantum mechanics. Engaging students with well-designed clicker questions is one of the commonly used research-based instructional strategies in physics courses partly because it has a relatively low barrier to implementation in classes of any size. Moreover, validated robust sequences of clicker questions are likely to provide better scaffolding support and guidance to help a variety of students build a good knowledge structure of physics than an individual clicker question on a particular topic. In this dissertation, I discuss a framework for the development, validation and in-class implementation of clicker question sequences (CQS) and apply that framework to help advanced undergraduate students learn quantum mechanics in the context of the Stern-Gerlach experiment, Larmor precession of spin, the addition of angular momentum, and the concepts involving Fermi energy and total electronic energy of a free electron gas and the Fermi-Dirac distribution function, several of which take advantage of the learning goals and inquiry-based guided learning sequences in previously validated Quantum Interactive Learning Tutorials (QuILT). The in-class evaluation of the CQSs using peer instruction is discussed. This dissertation also explores the impact of increased mathematical rigor in a QuILT on students' conceptual understanding of quantum optics. In particular, student performance after engaging with a QuILT, which uses a guided inquiry-based approach to help students learn concepts involved in a quantum eraser in the context of the Mach-Zehnder Interferometer (MZI), is

discussed for two versions: one version was primarily qualitative and the other involved both conceptual and quantitative aspects of the MZI. The implications of the extent to which students learned from the two versions of the QuILT within the Integration of Conceptual and Quantitative Understanding in Physics (ICQUIP) framework, which emphasizes appropriate integration of conceptual and quantitative aspects to equip students with functional knowledge and skills, are discussed. Finally, I discuss instructional pragmatism and how instructors should view teaching as a process and innovate in their courses using a variety of research-based instructional pedagogies to improve student learning.

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Preface

This dissertation embodies years of work that I could not have done without the assistance and support of many people. First and foremost, I want to thank Dr. Chandralkeha Singh. The impact of her role as my advisor cannot be understated. Without her tireless assistance, this undertaking truly would not have been possible.

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Finally, I thank my parents Tim and Sylvia Justice for making me who am I today, for loving me uncompromisingly, for nurturing my interest in science, and for showing me the stars.

1.0 INTRODUCTION

In physics education research (PER), a major goal is to help students build a robust knowledge structure and develop problem solving, reasoning and meta-cognitive skills. Evidence-based instructional methods are invaluable in accomplishing these goals for not only introductory physics students, but also for advanced physics students, such as those in upper-level quantum mechanics [1-39]. Within this dissertation, I investigate the efficacy of some of these evidence-based instructional methods in the context of learning quantum mechanics, which is a non-intuitive subject. In doing so, I explore the difficulties students exhibit with foundational concepts, determine ways in which these evidence-based instructional methods succeeded in addressing these difficulties, and propose strategies for improving those evidence-based instructional methods.

1.1 COGNITIVE SCIENCE

In order to help students build a robust knowledge structure and develop their reasoning and meta-cognitive skills in physics courses, cognitive science plays a central role in informing the development, validation and implementation of evidence-based instructional approaches and pedagogical tools. There are several cognitive models, described in this section, that were central throughout the development of the evidence-based instructional tools developed, validated and implemented as discussed throughout this dissertation.

1.1.1 Cognitive Apprenticeship Model

The Cognitive Apprenticeship Model is a field-tested model initially described by Collins, Brown, and Newman that focuses on how viewing helping students learn as an apprenticeship can help in creating effective learning environments [40]. This model involves three major components: modeling, coaching and scaffolding, and fading or weaning. In such a learning environment informed by the cognitive apprenticeship model, the instructor first demonstrates the criteria of good performance. This is followed by coaching and scaffolding which involves the instructor asking students to engage with tasks similar to the one that the instructor demonstrated and providing appropriate coaching and support. In other words, the instructor provides appropriate scaffolding support as students work on the task commensurate with their prior knowledge and similar to what has been modeled for them. Once students develop a certain level of proficiency, in the fading or weaning step of the cognitive apprenticeship model, the instructor gradually removes this scaffolding support until students develop self-reliance and can complete the task on their own. This cognitive apprenticeship model is different from the traditional instruction wherein elements of scaffolding or coaching are missing. In other words, students are lectured and instructor demonstrates what they want students to learn (even this modeling phase of the cognitive apprenticeship model is often not done very well in traditional instruction since instructors often think about the difficulty of concepts from their own perspective instead of from the perspective of the students they are teaching) and then students are asked to do their homework (in which students do not have sufficient opportunity to get support and feedback from their instructor or others, e.g., teaching assistants).

1.1.2 Piaget's Optimal Mismatch Model

Learning entails adapting one's knowledge structure via assimilation and accommodation. When one learns concepts and principles that are consistent with students' existing knowledge structure, it is called assimilation. However, when students learn concepts that highlight inconsistencies between what they are learning and their existing knowledge structure, it can cause a cognitive conflict or a state of disequilibrium. When this occurs, students may be motivated to accommodate that new information by changing or repairing their knowledge structure [41]. This accommodation is the core mechanism in Piaget's Optimal Mismatch Model, and allows students to discover mistakes in their own conceptual understanding via guided instruction and then opportunity to help them develop a robust knowledge structure.

1.1.3 Vygotsky's Zone of Proximal Development Model

Vygotsky's Zone of Proximal Development (ZPD) is the zone defined by what a student can do with the help of an instructor who is familiar with his/her prior knowledge and skills and uses this information to provide the student with appropriate guidance and support to learn as opposed to on his or her own [42]. In the ZPD, students can perform the tasks with the scaffolding support of the instructor but would not be able to do so without that support. As students gain higher level of mastery of the tasks and expand their conceptual knowledge structure, the ZPD expands, and student learning can be stretched further. If instruction is not within the ZPD but rather beyond it, learning will not be meaningful and students will struggle to develop a robust conceptual knowledge structure. If instruction is rote, students can perform associated tasks without support, and their knowledge structure has no opportunity to grow further. In contrast, instruction too far beyond students' current knowledge structure will be too difficult for them to benefit from even with instructor support. In this case, they will struggle less productively. By continuing to keep instruction within the ZPD, one can ensure that students can learn effectively.

1.1.4 Preparation for Future Learning

Bransford and Schwartz's Preparation for Future Learning (PFL) framework suggests that effective instruction should have elements of both innovation and efficiency [43]. If these elements are treated as orthogonal and plotted, an emphasis on efficiency would be represented by one axis, while an emphasis on innovation would be represented by the axis that is orthogonal to efficiency. If instruction is entirely focused on efficiency, students can become "rote experts," but their expertise is not adaptable to any other contexts. In contrast, instruction that is entirely focused on innovation provides students with little to no opportunity to practice the skills they are developing. In this framework, the most effective instruction includes both elements in what they call the Optimal Adaptive Corridor. Instruction in this region enables students to become adaptive experts who can transfer their knowledge to new domains readily.

1.2 PARADIGM SHIFT IN QUANTUM MECHANICS

This dissertation focuses on student learning of quantum mechanics. The diversity in student motivation, goals and prior preparation has increased significantly among physics majors. This makes teaching challenging for instructors. Moreover, the paradigm shift for upper-level students from classical mechanics to quantum mechanics can be particularly challenging [44]. For example, while students may have mastered classical mechanics, quantum mechanics is probabilistic rather than deterministic. This probabilistic nature of quantum mechanics is highlighted by the Heisenberg uncertainty principle, which necessitates that the more precisely the position of a particle is measured, the less precisely the momentum can be known.

This paradigm shift makes learning quantum mechanics even more challenging, analogous to the difficulties experienced by students in introductory physics who experience a paradigm shift from naïve conceptions of how things work to those learned in classical mechanics. In both cases, students lack familiarity with the new paradigm and hence are novices, even if they have developed expertise in another paradigm. This dissertation discusses development, validation and implementation of multiple evidence-based instructional pedagogies and how they guide students in building a hierarchical knowledge structure in this knowledge-rich domain of quantum mechanics.

1.3 CLICKER QUESTION SEQUENCES IN QUANTUM MECHANICS

This thesis consists of several studies pertaining to the development, validation, and evaluation of Clicker Question Sequences (CQS) on topics in upper level quantum mechanics. While a large number of physics instructors utilize clicker questions in their classrooms, little research has been done regarding development and validation of clicker question sequences in a synergistic way. In chapter 2, I present a framework for the development, validation and implementation of CQSs. Analysis of select CQSs is then discussed in chapters 2-5.

Engaging students with well-designed multiple-choice questions during class and asking them to discuss their answers with their peers after each student has contemplated the response individually can be an effective evidence-based active-engagement pedagogy in physics courses. Moreover, validated sequences of multiple-choice questions are more likely to help students build a good knowledge structure of physics than individual multiple-choice questions on various topics. Here we discuss a framework to develop robust sequences of multiple-choice questions and then use the framework for the development, validation and implementation of a sequence of multiple-choice questions focusing on helping students learn quantum mechanics via the Stern-Gerlach experiment (chapter 2), addition of angular momentum (chapter 3), Larmor precession of spin (chapter 4), and Fermi energy and total electronic energy of a free-electron gas (chapter 5) that takes advantage of the guided inquiry-based learning sequences in an interactive tutorial on the same topic. The extensive research in developing and validating the multiple-choice question sequence strives to make it effective for students with diverse prior preparation in upper-level undergraduate quantum physics courses. We discuss student performance on an assessment task focusing on these topics after traditional lecture-based instruction vs. after engaging with the research-validated multiple-choice question sequence administered as clicker questions in which students had the opportunity to discuss their responses with their peers.

Instructional pragmatism is essential for successfully adopting and adapting evidence-based active engagement (EBAE) approaches in that instructors should view improving teaching and learning as a process and not get disheartened if a particular EBAE approach does not produce the desired outcome. Instructional pragmatism entails keeping a variety of EBAE methods in one's instructional toolbox and using them flexibly as needed to improve student learning and continuously refining and tweaking one's implementation of the EBAE approaches to make them effective. Here we illustrate an example of instructional pragmatism in which a quantum mechanics instructor did not give up when an EBAE method involving implementation of a sequence of clicker questions on addition of angular momentum did not yield expected learning outcomes even though it was found effective earlier. Instead, the instructor remained optimistic, viewing improving teaching and learning as a process, and pulled out another EBAE method from his tool box that did not require him to spend more time on this topic in class. In particular, the instructor created an opportunity for students to productively struggle with the same problems they had not performed well on by incentivizing them to correct their mistakes out of class. Student performance on one of the addition of angular momentum problems posed on the final exam suggests that students who corrected their mistakes benefited from the task and learned about addition of angular momentum better than those who did not correct their mistakes. Encouraging and supporting physics instructors to embrace instructional pragmatism can go a long way in helping students learn physics because it is likely to increase their persistence in using various EBAE approaches flexibly as they refine and tweak their implementation for their students. This is discussed in chapter 3.

I conducted an investigation of the difficulties that undergraduate physics students in upper-level quantum mechanics and graduate students have with Fermi energy, the Fermi-Dirac distribution, and total electronic energy of a free electron gas after quantum and statistical mechanics core courses. These difficulties were probed by administering written conceptual and quantitative questions to undergraduate students and asking some undergraduate and graduate students to answer those questions while thinking aloud in one-on-one individual interviews. We find that advanced students have many common difficulties with these concepts after traditional lecture-based instruction. Engaging with a sequence of clicker questions improved their performance, but there remains room for improvement in their understanding of these challenging concepts. This is discussed in chapter 5.

1.4 FURTHER CQS CONSIDERATIONS

In addition to the CQSs presented in chapters 2-5, I have helped develop CQSs on a number of other topics in quantum mechanics. A selection of these are included in Appendix A alongside those discussed and analyzed in chapters 2-5.

1.5 IMPACT OF ADDING MATHEMATICAL RIGOR TO QuILT

We use the "Integrating Conceptual and Quantitative Understanding In Physics" or "ICQUIP" framework to develop, validate and evaluate a Quantum Interactive Learning Tutorial (QuILT) which incorporates mathematical rigor while focusing on helping students develop expertise, i.e., a good conceptual understanding of quantum optics using a Mach Zehnder Interferometer with single photons and polarizers. We compare upper-level undergraduate and graduate students' performance on conceptual questions after engaging with this "hybrid" (conceptual and quantitative) QuILT with a conceptual QuILT focusing on the same topics in which quantitative tools were not employed. Both versions of the QuILT use a guided inquiry-based approach to learning and are based on research on student difficulties in learning these challenging concepts as well as a cognitive task analysis from an expert perspective. The hybrid and conceptual QuILTs were part of the courses for upper-level undergraduates or first year physics graduate students in several consecutive years at the same university. Although the course instructors were different, the same individual facilitated the in-class hybrid or conceptual QuILT in all of the courses as a guest instructor to maintain uniformity in implementation. We find that physics graduate students' posttest performance on *conceptual* questions after engaging with the hybrid QuILT was generally better than their performance after engaging with the conceptual QuILT. For undergraduate students, the results were mixed. In particular, one group of undergraduates, which had roughly a 50% average pretest score after traditional lecture-based instruction on these topics and which engaged with the hybrid QuILT after the pretest, outperformed the undergraduates who engaged with the conceptual QuILT on the posttest, which was completely conceptual. On the other hand, another group of undergraduates, which had roughly a 25% average pretest score after traditional lecture-based instruction on these topics and which engaged with the hybrid QuILT after the pretest, had reasonable posttest performance on some conceptual questions, especially those pertaining to two-dimensional Hilbert space involving only path states (no polarization states of single photons involved since polarizers were not present in those experimental situations). However, their performance on many of the other conceptual posttest questions was worse than that of the undergraduates who used the conceptual QuILT. One possible interpretation of these findings consistent with the ICQUIP framework is that integration of conceptual and quantitative aspects of physics should be commensurate with students' prior knowledge of relevant physics and mathematics so that students do not experience cognitive overload while engaging with such a learning tool striving to develop a good grasp of physics concepts. In the undergraduate course in which students did not benefit as much from the hybrid QuILT that focused on integration of conceptual and quantitative understanding to help students learn physics concepts, their pretest performance suggests that the traditional instruction may not have sufficiently given a "first coat" and prepared students with requisite physics concepts to engage with the hybrid QuILT. Since physics majors in the required undergraduate quantum mechanics course come with diverse physics and mathematics backgrounds, the hybrid QuILT may have caused cognitive overload at least for some students (on topics in which their conceptual posttest performance is not good) so that they could not benefit from integrated conceptual and quantitative learning sequences. In other words, integration of conceptual and quantitative understanding in physics must adequately build on students' prior knowledge to avoid cognitive overload and help students develop expertise. This is discussed in chapter 6.

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2.0 IMPROVING STUDENT UNDERSTANDING OF QUANTUM MECHANICS UNDERLYING THE STERN-GERLACH EXPERIMENT USING A RESEARCH-VALIDATED MULTIPLE-CHOICE QUESTION SEQUENCE

2.1 INTRODUCTION

2.1.1 Background

A major goal of many physics courses from introductory to advanced levels is to help students learn physics concepts [1-7] while also helping them develop problem solving and reasoning skills [8-18]. We have been investigating strategies to help students develop a solid grasp of physics concepts and develop their problem solving and reasoning skills [19-31]. In fact, many education researchers have been involved in developing and evaluating evidence-based active-engagement (EBAE) curricula and pedagogies [32-50], but implementation of these EBAE approaches to help college students learn has been slow. Some of the major barriers to implementation of the EBAE pedagogies at the college-level include lack of faculty buy-in and their reluctance and/or resistance, partly due to a lack of institutional reward system for using these evidence-based approaches, the time commitment involved in effectively adapting and implementing them, and instructors' fear that their students may complain (since students may prefer to passively listen to lectures as opposed to actively engage in the learning process) [32].

2.1.2 Use of Multiple-Choice questions and peer interaction

The use of well-designed multiple-choice questions in the classroom in which each student must first take a stand before discussing the responses with peers is an EBAE pedagogy that has a relatively low barrier to implementation. These multiple-choice questions can be used in a variety of ways to engage students actively in the learning process. For example, "think-pair-share" approach in which each student thinks about why a particular answer choice is correct for each question first and then pairs up with a peer sitting next to them to share their thoughts before a general discussion about the correct answer can be an effective pedagogy. The use of multiple-choice questions keeps students focused during the lectures and helps them self-monitor their learning. Moreover, depending upon instructional goals and instructors' preferences, multiple-choice questions can be used in diverse manner, e.g., they can be interspersed within lectures to assess student learning of the material in each segment, posed at the end of a class or used to review materials from previous classes. They can be used in a flipped class in which the class time is entirely focused around multiple-choice questions and discussions around them [32].

Integration of peer interaction with lectures using multiple-choice clicker questions has been made popular by Mazur in the physics community [33]. In Mazur's approach, the instructor poses conceptual, multiple-choice clicker questions to students throughout the class. Students first answer each multiple-choice question individually using clickers (or personal response system), which requires them to take a stance regarding their understanding of the concepts involved [33]. Next, they discuss the questions with their peers and learn by articulating their thought processes and assimilating their ideas and understanding with those of the peers. Then, there is a class discussion involving all students about those concepts in which both students and the instructor participate fully. By having students take a stand anonymously using clickers as opposed to using a show of hand for each answer choice selected for a multiple-choice question, students do not feel embarrassed if their answer choices are not correct. Moreover, clickers offer another advantage over a show of hand or show of cards with different colors (for different answer choices selected for each multiple-choice question) in that the responses are recorded and the instructor can contemplate how to address the common difficulties that students have (which they otherwise may not feel comfortable sharing with the instructor). In particular, the immediate feedback that is obtained by the instructors is valuable because they have an understanding of the extent of student difficulties and the percentage of students who understand the concepts.

2.1.3 Multiple-Choice Question Sequences

While multiple-choice questions, which can be used with or without clickers, have been developed [33-45] for introductory physics and upper-level physics such as quantum mechanics (QM), there have been very few documented efforts [45] toward a systematic development of multiple-choice question sequences (MQSs) in which the set of questions build on each other effectively and help students extend, organize and repair their knowledge structure. Moreover, in the past two decades, many investigations have focused on improving student learning of QM, e.g., see [51-64]. Our group has been involved in such investigations and we are using the research on student difficulties as a guide to develop research-validated learning tools [65-84]. Our past investigations in upper-level QM courses suggest that while engaging students with multiple-choice questions during class can help them learn, they may not be as effective as a research-validated QuILT on the same concepts unless they are carefully sequenced [68]. For example, we find that when students in upper-level undergraduate QM course only had traditional lecture-based instruction, their performance on a quantum measurement quiz covering those concepts was 26%

[68]. The next year, the student performance in the same course on an equivalent quiz on quantum measurement concepts was 68% after lecture and multiple-choice questions on quantum measurement, and their score on another equivalent quiz was 91% after engaging with a QuILT on quantum measurement [68]. A research-validated MQS has the potential to bridge the gap between students' performance after they engage with a QuILT vs. after they engage only with a MQS on the same topic (since the multiple-choice questions in a MQS build on each other and can take advantage of the learning objective and guided sequences in the corresponding QuILT).

Here we discuss a framework for the development, validation and implementation of a MQS and then apply it to develop and validate a MQS to help students learn about Stern-Gerlach experiment, a topic which is valuable for exposing students to the foundational issues in QM, by taking advantage of the guided learning sequences in a research-validated Quantum Interactive Learning Tutorial (QuILT) on that topic [66]. The SGE MQS strives to help students learn fundamental issues in QM using a simple two-state system. We also discuss the implementation of this MQS by two different instructors using clickers with peer discussions interspersed throughout the class. A QuILT focusing on a QM concept uses a guided, inquiry-based approach to learning and consists of learning sequences, which are based both upon a cognitive task analysis from an expert perspective and an extensive research on student difficulties in learning those concepts. The QuILT was useful both for developing new multiple-choice questions and revising/fine-tuning existing multiple-choice questions (e.g., in situations in which individual multiple-choice questions are already validated but the sequencing of questions is not validated), or for developing entirely new multiple-choice questions to ensure that different questions in the MQS build on each other. Before we focus on a MQS that strives to help students learn about the Stern-Gerlach experiment (SGE), we enumerate the learning objectives.

2.1.4 Learning objectives of the SGE MQS

The learning objectives of the SGE MQS are commensurate with the corresponding QuILT [66], which guided the development and sequencing of the SGE MQS questions. These learning objectives are focused on improving student understanding of the foundational issues in QM via the Stern-Gerlach experiment and were developed using extensive research on student difficulties with these concepts and cognitive task analysis from an expert perspective [66]. These foundational issues include the difference between the physical space (in which the experiment is performed) and the Hilbert space (in which the state of the quantum system lies), quantum state preparation, quantum measurement and the difference between a superposition and mixture. We find that after traditional lecture-based instruction, many students have difficulty differentiating between the physical space and Hilbert space. For example, they believe that if a neutral silver atom in an eigenstate $|\uparrow\rangle_x$ of the *x* component of the spin angular momentum $\hat{S}_x$ is sent through a Stern-Gerlach apparatus (SGA) with magnetic field gradient in the *z* direction, the magnetic field will not impact the quantum state because the magnetic field gradient is orthogonal to the quantum state $|\uparrow\rangle_x$. This type of reasoning is incorrect because the quantum state is a vector in the Hilbert space in which the state of the system lies whereas the magnetic field is a vector in the physical space in which the experiment is being performed. It does not make sense to talk about orthogonality of two vectors in different vector spaces. Thus, the first learning objective of the MQS is to help students develop a solid grasp of the difference between the physical space and Hilbert space using the SGE with a two state system as an example. The second learning objective focuses on helping students develop a functional understanding of quantum state preparation because one fundamental issue that the SGE can beautifully illustrate at least conceptually using a two state system is the issue of how to prepare a quantum state. For example, if a quantum system consisting of a large number of neutral silver atoms is initially in an eigenstate $|\uparrow\rangle_z$ of the z component of the spin angular momentum $\hat{S}_z$, is it possible to use appropriate SGAs and detectors to prepare a state which is orthogonal to it, i.e., $|\downarrow\rangle_z$? The third learning objective focuses on helping students learn about quantum measurement in the context of a simple two-state system (e.g., using a beam of neutral silver atoms which can be treated as a spin-1/2 system) in a given spin state and how the state of the silver atoms is impacted by passing through a SGA and how the placement of the detectors (that can detect the silver atoms) in appropriate positions will collapse the state to different eigenstates of the observable measured with different probabilities, depending upon the set up. The fourth learning objective is to help students understand that there is a difference in the situations in which a beam of silver atoms propagates through a series of SGAs but no measurement via a detector is performed vs. the case in which a detector is present for measuring the silver atoms deflected upward or downward (because the measurement will collapse the state of the system into an eigenstate of the measured observable with different probabilities). Since the orbital and spin degrees of freedom of the silver atoms are entangled, a detector after a SGA in the up channel or down channel clicking would signify the spin state of the silver atom collapsing to a particular state. The fifth learning objective is to help students be able to analyze the probabilistic outcome of a measurement when a given initial two-state system is sent through a SGA by transforming the initial state given in a basis to another basis that is more suited for the analysis of measurement outcomes based upon the magnetic field gradients (e.g., if the Stern-Gerlach apparatus has a gradient in the *x* direction, the most convenient basis in which the incoming state should be transformed to analyze the measurement outcomes consists of eigenstates of the x component of the spin angular momentum). Finally, the sixth learning objective of the MQS is to help students be able to develop a functional understanding of the difference between a superposition vs. mixture and how certain experimental configurations involving SGAs are able to differentiate between them.

2.2 METHODOLOGY FOR DEVELOPING, VALIDATING, AND IMPLEMENTING A MQS

Before discussing the SGE MQS, we first summarize general issues involved in the development, validation and implementation of a robust MQS using the inquiry-based learning sequences in the corresponding QuILT as a guide. In particular, below, we summarize some of these "lessons learned" from the guided sequences in the QuILT that can be used as a guide to develop and/or revise a MQS (first three points below) and implement it effectively (last three points below:

2.2.1 Balance difficulty

A QuILT is structured such that students are provided enough guidance to develop a coherent conceptual understanding without becoming frustrated or discouraged. Following this principle and earlier suggestions to make effective use of class time, e.g., by Mazur et al. [33], we decided that a majority of the questions in a MQS should have correct response rates such that both extremes are avoided (i.e., we avoided cases in which very few students answer the question correctly or incorrectly). If some students already have a reasonable understanding of the topic, it is likely to make the peer discussions effective and encourage students to engage in productive discussions and learn the concepts with peer support. A question in which very few students can reason about it correctly may result in reinforcing students' inaccurate conceptual models and it also becomes more likely that students would guess as opposed to apply the physics concepts systematically. On the other hand, high scores indicate that there is little constructive struggle. With restricted class time, such questions should be limited except for warmups (to help students review basic concepts and prime them to answer more complex questions later) [45].

2.2.2 Change only the context or the concept between questions

We took inspiration from the corresponding QuILT [66] on the same topic to ensure that different questions in the MQS build on each other and ascertain how changes in context and concepts should be included in the MQS. We found that switching both the concept and the context in adjacent questions may result in cognitive overload for students. Changing only the context or concept between consecutive questions may help students identify the differences and similarities between subsequent questions and construct correct models more effectively.

2.2.3 Include a mix of abstract and concrete questions

Although the type of questions in a MQS is usually dictated by the topic and the goals and learning objectives, we examined guided learning sequences in the QuILT [66] to determine how to pose abstract and concrete questions in a MQS. Abstract questions may provide students opportunities to generalize concepts across different contexts. On the other hand, concrete questions allow students to apply their learning to a concrete context. Students may benefit from a balance of both question types.

2.2.4 Allow student collaboration

Collaborative group work is found to be beneficial for helping many students learn [33-50]. A student who is having difficulty and a student who is articulating her thoughts both refine their understanding so that co-construction of knowledge can occur when neither student was able to answer the questions before peer collaboration, but were able to answer them correctly after working together [33]. Thus, instructors should allow for peer discussion while implementing a MQS.

2.2.5 Incorporate "checkpoints" at appropriate times during a MQS

A QuILT often includes checkpoints which provide opportunity to reconcile the differences between student ideas and the correct conceptual model. The MQS for a given topic can include "checkpoints" at similar points as the QuILT, at which the instructor can have a general class discussion and can give feedback to the entire class based upon students' multiple-choice question responses to help them learn.

2.2.6 Include a manageable number of multiple-choice questions per sequence

The researchers deliberated and concluded (based upon data from multiple-choice questions in previous years and the learning sequences in the QuILT) that a MQS should include a manageable number of questions that should build on student prior knowledge. Having many questions in a sequence may offer students more opportunities to practice concepts, but having too many questions can result in a sequence of multiple-choice questions that cannot be reasonably implemented effectively, given the time constraints of the class.

2.3 METHODOLOGY FOR DEVELOPING AND VALIDATING SGE MQS

In order to develop and validate effective sequences of multiple-choice questions for QM focusing on the SGE, three researchers met to holistically examine the instructional materials from the past few years on these topics in an upper-level undergraduate QM course at a large research university in the US, which included existing multiple-choice questions and the QuILT on this topic. This course typically has 15-25 students each year, who are mainly physics juniors/seniors. The validation of MQS was an iterative process. Moreover, the questions in the SGE MQS were developed or adapted from prior validated multiple-choice questions and sequenced to balance difficulties, avoid change of both concept and context between adjacent questions as appropriate in order to avoid experiencing cognitive overload, and include a mix of abstract and concrete questions to help students develop a good grasp of the concepts. In particular, in order to design an effective SGE MQS, we examined the SGE QuILT [66] and contemplated how to take advantage of its learning objectives, guided learning sequences, and student performance on the pre-/posttests administered before and after they engaged with it.

While developing the SGE MQS, we drew upon the learning objectives delineated earlier and the requisite knowledge and skills required to achieve those objectives. We also focused on the order in which different QM concepts that are involved in the learning objectives are invoked and applied in a given situation within the SGE QuILT to inform the design of the SGE MQS. Furthermore, we carefully examined the types of scaffolding provided in the SGE QuILT [66] to reflect on how different questions within the SGE MQS should effectively build on each other and whether more scaffolding between some existing multiple-choice questions is required. We also analyzed student performance on SGE multiple-choice questions in previous years to determine whether students were able to transfer their learning from one multiple-choice question to another and whether some multiple-choice questions would require more scaffolding between them in order to be effective. In particular, when examining the SGE MQS that had been administered in the previous years and comparing them with the guided learning sequences in the SGE QuILT, we realized that sometimes both the concept and the context changed from the preceding to the following question in an old sequence. We hypothesized that this may cause cognitive overload for students and at least partly be responsible for making the previous set of multiple-choice questions less effective (for which we had evidence from the data from previous years). We took inspiration from the SGE QuILT to develop the set of questions for the SGE MQS that have appropriate ordering and balance to scaffold student learning and help them compare and contrast different concepts and contexts effectively. The issue of abstract vs. concrete questions was also deliberated. Abstract questions posed tend to focus on generalized cases whereas concrete questions, in general, involve a specific context. It was decided that only the last question in the MQS will have an abstract choice since the SGE is best learned using concrete examples using diverse setups of SGAs and initial states.

After the initial development of the SGE MQS using the learning objectives, inquiry-based guided sequences in the QuILT and existing individually validated questions, we iterated the MQS with three physics faculty members who provided valuable feedback. The feedback from faculty helped in fine-tuning and refining some new questions that were developed and integrated with the existing ones to construct the sequence of questions in the SGE MQS and to ensure that the questions were unambiguously worded and build on each other based upon the learning objectives. We also interviewed four students individually who answered the MQS questions in a one on one interview situation while thinking aloud so that we could understand their thought processes. The four interviews totaled about 3 hours. These interviews, which also reaffirmed the common difficulties earlier described by Zhu et al. [66], ensured that students found these questions unambiguous and were able to take advantage of the scaffolding provided by different questions that build on each other. These student interviews were helpful for further tweaking the questions.

2.4 MQS FOCUSING ON THE SGE THAT WAS IMPLEMENTED IN CLASS

After the out-of-class development and validation, the final version of the SGE MQS that went through in-class implementation via clickers along with peer discussion has 7 questions (MQ1-MQ7). As discussed in the next section, two different instructors at the same institution implemented the SGE MQS in two consecutive years in the upper-level undergraduate QM course such that the pretest was given after traditional lecture-based instruction, and then students engaged with the entire SGE MQS with 7 questions in class before they were administered the posttest. There was no overall class discussion after MQ1 but there was an overall class discussion after each of the other questions in the SGE MQS.

Similar to the QuILT [66], in the MQS administered as clicker questions with peer interaction and the corresponding pretest and posttest, the description of the Stern-Gerlach apparatus shown in Figure 2.1 was provided to students because it is important to clarify the notation used for the SGAs. Students also knew that the orbital angular momentum of a beam of neutral silver atoms is zero, so they had to focus on the fact that a beam of neutral silver atoms passing through a SGA can be considered a spin-1/2 system. They had learned that a SGA can entangle the orbital and spin degrees of freedom depending upon the initial state of the system and the SGA setup. Students also were asked to assume that the detectors were placed in appropriate orientations after a SGA and when a detector clicks, the silver atom is absorbed by that detector.

The figure below shows the pictorial representations used for a Stern-Gerlach apparatus (SGA). If an atom with state $|\uparrow\rangle_z$ *(or* $|\downarrow\rangle_z$*) passes through a Stern-Gerlach apparatus with the field gradient in the negative z-direction (SGZ-), it will be deflected in the +z (or -z) direction. If an atom with state* $|\uparrow\rangle_z$ *(or* $|\downarrow\rangle_z$*) passes through a Stern-Gerlach apparatus with the field gradient in the positive z-direction (SGZ+), it will be deflected in the -z (or +z) direction. Similarly, if an atom with state* $|\uparrow\rangle_x$ *passes through SGX- (or SGX+), it will be deflected in the +x (or -x) direction. The figures below show examples of deflections through the SGX and SGZ in the plane of the paper. However, note that the deflection through a SGX will be in a plane perpendicular to the deflection through an SGZ. This actual three-dimensional nature should be kept in mind in answering the questions.*

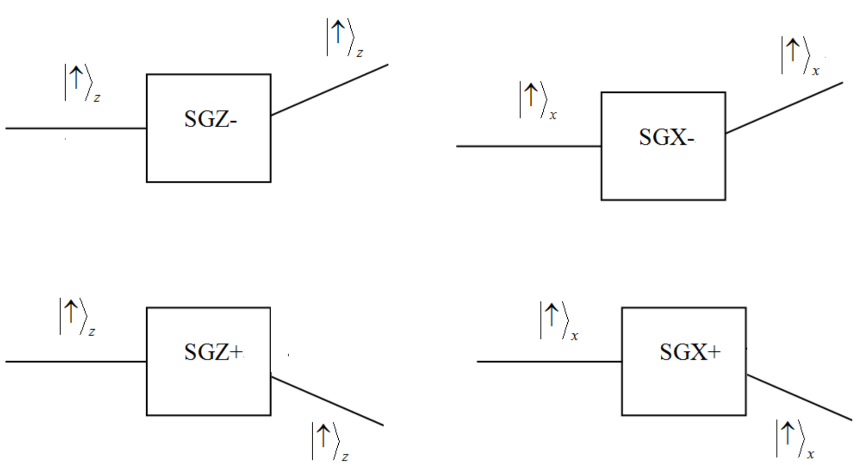

Figure 2.1 This information is provided to students in all contexts (e.g., before the MQS and with the pretest and posttest).

The first two questions of the MQS, questions MQ1 and MQ2, focus on student difficulty in differentiating between Hilbert space and physical space as well as on the choice of an appropriate basis to analyze the probability of measuring different outcomes given a particular initial state of the system and the SGE setup as follows. Correct answers are in bold for all multiple-choice questions.

(MQ1) *A beam of neutral silver atoms in a spin state* $|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_z + |\downarrow\rangle_z)$ *propagates into the screen (x-direction) as shown in Figure 2.2. The beam is sent through a SGE with a horizontal magnetic field gradient in the* <u>*–z-direction*</u>*. What is the pattern you predict to observe on a distant screen in the y-z plane when the atoms hit the screen?*

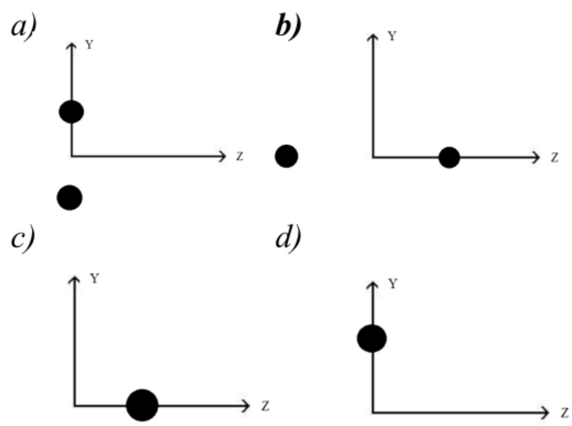

Figure 2.2 Figure for MQ1

(MQ2) *A beam of neutral silver atoms in a spin state* $|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_z + |\downarrow\rangle_z)$ *propagates into the screen (x-direction) as shown in Figure 2.3. The beam is sent through a SGE with a horizontal magnetic field gradient in the* <u>*–y-direction*</u>*. What is the pattern you predict to observe on a distant screen in the y-z plane when the atoms hit the screen?*

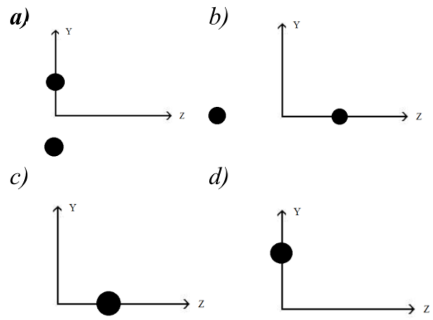

Figure 2.3 Figure for MQ2

In the in-class administration discussed in the next section, after students answered both questions using clickers after discussing their responses with a peer sitting next to them, a whole class discussion led by the instructor focused on common student difficulties, e.g., in differentiating between physical space and Hilbert space, the importance of choosing an appropriate basis and transforming the initial state in that basis in order to analyze the measurement outcomes before posing MQ3 as a clicker question. In question MQ3 (see Appendix II), students were told that $|a|^2+|b|^2=1$. In MQ3, silver atoms in a generic spin state given in the basis of eigenstates of $\hat{S}_z$ are sent through a single Stern-Gerlach apparatus with an *x* gradient. This question focuses on helping students learn about the usefulness of transforming from the given basis to a more suitable basis in order to analyze the measurement outcomes including the probability of the detector clicking. It also helps students learn about preparing a specific spin state, here $|\downarrow\rangle_x$. Building on this question, MQ4-MQ6 (see Appendix II) ask students to contemplate issues related to preparation of quantum states in different arrangements of SGAs and initial state. In MQ5, students were told to assume that the strength of the second SGA was such that any spatial separation of the state after the first SGA was negated. Finally, MQ7 focuses on helping students think about how to use the SGE to differentiate between a state which is a superposition of eigenstates of an operator corresponding to an observable and a mixture. We note that oblique lines are shown as a guide only in some of the figures (e.g., Figures 2.7, 2.8 and 2.9) as a scaffolding support but not shown in others, e.g., in Figures 2.6 and 2.11 so that students learn to think about and draw them themselves. We also note that there are many experimental considerations in constructing a real SGA, e.g., the challenge of maintaining coherence between two spatially separated beams such as in MQ5. These considerations were not discussed by the instructor (since it has the possibility to increase student cognitive load) but would certainly add richness to the topic.

2.5 METHODOLOGY FOR IN-CLASS IMPLEMENTATION

Not only did we focus on developing and validating the SGE MQS, we also contemplated effective strategies for their in-class implementation. For example, we used the SGE MQS with clickers and peer discussion, a principle emphasized by Mazur [33]. In fact, empirical data from QM multiple-choice questions given in previous years suggest that, on average, student performance on multiple-choice questions improved significantly after discussing responses with a peer [35]. We also considered the need for productive struggle for students when working on the SGE MQS. For example, we considered the points at which the instructor should provide feedback to students in order to maximize productive engagement and minimize discouragement. Again we drew both upon the SGE QuILT and empirical data from student responses to multiple-choice questions in previous years to identify where feedback might be most effective in the SGE MQS. We paid attention to the QuILT "checkpoints" for students to resolve possible conflicts between their understanding and the correct conceptual model of the foundational issues elucidated via the SGE [66]. These "checkpoints" guided us in identifying points for instructor feedback and general class discussion for the SGE MQS that may be beneficial for students. We also analyzed the points at which students struggled when answering clicker questions in previous years to determine possible points during the implementation of the SGE MQS when a particular general class discussion was likely to be effective. It was determined that one productive approach would be for the instructor to have students answer the first two SGE MQS questions before having a general class discussion followed by a class discussion after each of the following SGE MQS questions.

We note that the final version of the 7 SGE MQS questions can be integrated with lectures in which these relevant concepts pertaining to SGE are covered in a variety of ways based upon the instructor's preferences. For example, the MQS can be given over multiple sessions or together depending, e.g., upon whether these are integrated with lectures, used at the end of each class, or used to review concepts after students have learned about the Stern-Gerlach experiment via lectures. However, in this study, the SGE MQS was implemented with clickers and peer discussion [33] in an upper-level undergraduate QM class at a large research university after traditional lecture-based instruction in relevant concepts on the Stern-Gerlach experiment for two consecutive years by two different instructors. Both instructors tried their best to implement the SGE MQS in a very similar manner using clickers and peer discussion and with similar general whole class discussions that was deemed effective as discussed in the preceding paragraph. Prior to the implementation of the SGE MQS in class, students were administered a pretest after traditional lecture-based instruction, which was developed and validated by Zhu et al. [66] to measure comprehension of the relevant concepts. The students then engaged in class with the SGE MQS and discussed their answers with their peers. This implementation was completed in one class period. The posttest was administered during the following week to measure the impact of the SGE MQS on student learning of relevant concepts.

The posttest that students were administered following the implementation of the SGE MQS was analogous to the pretest [66]. These pre-/posttests are the same as those administered by Zhu et al. to measure student learning after traditional lecture-based instruction and after engaging with the SGE QuILT [66]. In order to compare the performance of the SGE MQS and QuILT groups on pre-/posttests so that the relative improvements can be determined, the same rubric was used for the pre-/posttests given to the SGE MQS students as the corresponding QuILT students in Ref. [66] (who were also advanced undergraduate students in QM course at the same university). All questions were scored out of a possible 2 points, with partial credit assigned to answers that were correct, but for which either incorrect justification or no justification was provided if reasoning was requested. The inter-rater reliability was better than 95%.

We also note that two versions (test versions A and B) of the tests were designed to be administered as a pretest or posttest. In particular, all questions on the two versions of the test are not identical because we wanted to investigate how students answer questions when the pretest and posttest questions are the same or different. Moreover, the version of the test that was used as a pretest before the SGE MQS in one year was used as a posttest in the other year. The first two questions in the pretest and posttest are analogous to MQ1 and MQ2 in the SGE MQS. Question 1 on both versions is identical and pertains to a state, which is an equal superposition (no relative phase factor) of the spin-up and spin-down states in the z-basis, passing through a SGE with a magnetic field gradient in the -*z* direction (identical to MQ1). Question 2 has silver atoms with spin-up in the z-basis passing through a SGE with a magnetic field gradient in either the -*y* direction (as in MQ2) or –*x* direction, depending on the version of the test. These first two questions address the first learning objective. Question 3 on both versions of the test corresponds to MQ3. On both versions A and B of the test (see Appendix III), question 3 asks about the measurement outcomes for a superposition of spin-up and spin-down states in the z-basis passing through a SGX-. On version A, both coefficients of the state are given numerically, whereas they are given in terms of complex numbers "a" and "b" in version B with $|a|^2+|b|^2=1$. This question addresses both the third and fifth learning objectives.

Question 4 on both versions most closely matches MQ4, but also connects with MQ5 and MQ6. The question 4 in version B is shown in Figure 2.11 in Appendix III. On version A, the first SGE seen in MQ4 is a SGY-, rather than SGX-. On version B, there is an additional SGZ- in front of the SGX-. This question emphasizes the second learning objective, while also addressing the third, fourth, and fifth learning objectives.

Question 5 on test version A and the analogous test question on version B align with the learning objectives underlying MQ7, i.e., they assess whether students are able to differentiate between a superposition state and an analogous mixture using SGAs. In both versions (see Appendix III), students are given two beams of silver atoms: a superposition $|\chi\rangle = \sqrt{\frac{1}{2}}|\uparrow\rangle_z + \sqrt{\frac{1}{2}}|\downarrow\rangle_z$, and the analogous mixture of 50% $|\uparrow\rangle_z$ and 50% $|\downarrow\rangle_z$. Version A asks students to design a setup of SGAs to differentiate between these two beams (superposition and mixture), while version B asks students to identify which combination of three statements is true regarding these beams passing through different SGAs (see Appendix III). This question emphasizes the sixth learning goal, while also addressing the third and fifth.

Finally, on the same topic as question 4, question 6 (see Appendix III) on both versions of the test assesses student understanding of preparing a state (here students are given an initial state and asked if they can prepare a given orthogonal state using SGAs and how they may be able to do that), and connects most closely with MQ6 asking students to design a setup of SGAs to prepare a spin-up state in the *z*-basis given an initial spin-down state in the *z*-basis. This question emphasizes the second learning objective, while also addressing the third, fourth, and fifth.

2.6 IN-CLASS IMPLEMENTATION RESULTS

In one year of the SGE MQS implementation in upper-level undergraduate QM, students were administered version A as a pretest and version B as a posttest, while in the other year, they were administered version B as a pretest and version A as a posttest. On the other hand, when the SGE QuILT was implemented [66], some of the students in the same class were given version A as the pretest whereas others were given version B (and the versions were switched for each student for the posttest). Tables 2.1 and 2.2 compare pre-/posttest performances of students in upper-level QM course from the same university in different years after traditional lecture-based instruction (pretest) and on the posttest after students had engaged with the SGE MQS (Table 2.1) or SGE QuILT (Table 2.2). The normalized gain (or gain) is calculated as $g = (post\% - pre\%)/(100\% - pre\%)$ [85]. Effect size was calculated as Cohen's $d = (\mu_{post} - \mu_{pre})/\sigma_{pooled}$ where μ_i is the mean of group *i* and where the pooled standard deviation (in terms of the standard deviations of the pre- and posttests) is $\sigma_{pooled} = \sqrt{\sigma_{pre}{}^2 + \sigma_{post}{}^2/2}$ [85]. Normalized gain and effect size are only shown in Table 2.1 (not available for Table 2.2 data in Ref [66]).

Table 2.1 Comparison of the mean pre/posttest scores on each question, normalized gains and effect sizes for students in upper-level undergraduate QM (averaged over two years in which the corresponding questions in versions A and B are averaged) who engaged with the SGE MQS (N=48).

Question	Pretest Mean	Posttest Mean	Normalized Gain (g)	Effect Size (d)
1	61%	96%	0.88	0.50
2	40%	92%	0.87	0.71
3	38%	49%	0.18	0.13
4	51%	80%	0.59	0.38
5	24%	50%	0.34	0.28
6	43%	82%	0.69	0.46

Table 2.2 Comparison of mean pre/posttest scores on each question from Ref. [66] (effect sizes not available) for students in upper-level undergraduate QM who engaged with the SGE QuILT. Questions from versions A and B were mixed in both pre- and posttest in that some students got version A as the pretest and others as the posttest (and vice versa). Mean scores are not for matched students and numbers of students varies from 5 to 35 (more details can be found in Ref. [66]).

Question	Pretest Mean	Posttest Mean
1	80%	81%
2	39%	77%
3	30%	80%
4	40%	90%
5	42%	90%
6	38%	100%

Tables 2.1 and 2.2 show that students in general did not perform well on the pretest after traditional lecture-based instruction. Note that we have combined the data for questions which have been treated as equivalent between versions A and B, whereas Zhu et al. refer to questions from different versions separately in Ref.[66].

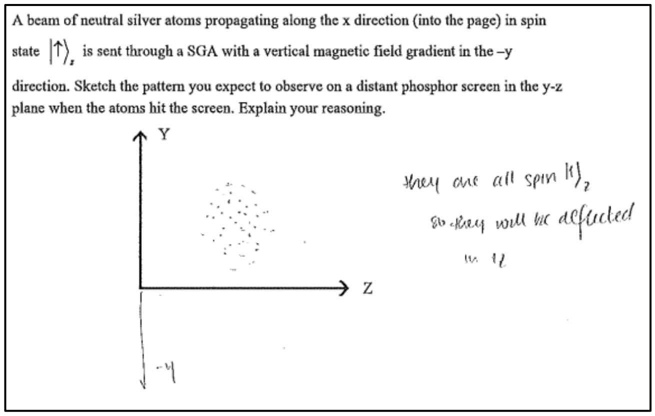

Figure 2.4 An example of a common student belief that the state of the beam propagating through the Stern-Gerlach apparatus will be deflected in the z direction because the state is $|\uparrow\rangle_z$ in response to question 2 on version B of the test.

However, Table 2.1 shows that there is significant improvement on the first two questions from the pretest (after traditional lecture-based instruction in relevant concepts) to posttest (after the SGE MQS) with students using the SGE MQS scoring greater than 90% on both questions. This improvement in students' understanding is partly due to students being able to differentiate between the Hilbert space and physical space better and also being able to choose a suitable basis for the initial state of the system sent through a SGA and analyze the outcomes of an experiment based upon the magnetic field gradient of the SGA after engaging with the SGE MQS.

Switching between bases and preparation of a state orthogonal to an initial state are investigated via test questions 4 and 6 (see Figure 2.3) and MQ4. Table 2.1 also shows that on both questions 4 and 6, there was a reasonable gain from pretest to posttest after the SGE MQS implementation. While not as large as the gains observed for these questions from pretest to posttest for students using the SGE QuILT (see Table 2.2), Table 2.1 shows that students scored approximately 80% in response to these questions after engaging with the SGE MQS (these questions were about a situation in which the final prepared spin state of the silver atoms was a "flipped" state orthogonal to the spin state of the incoming atoms, and a situation in which students had to design an experiment with a series of SGAs with the goal of "flipping" the incoming quantum state).

In contrast, questions 3 and 5 both demonstrate some room for improvement on posttest even after the SGE MQS implementation (see Table 2.1) compared to the corresponding improvement after the SGE QuILT (see Table 2.2). An example of a student response to Question 3 on the pretest on version A is shown in Figure 2.5, in which the student had difficulty recognizing that the initial state is an eigenstate $|\uparrow\rangle_x$ of $\hat{S}_x$ so the entire beam will be deflected upward in this situation. The student stated that the probability of the detector clicking when an atom exits the SGX- is *"50% probability because the SGE is in the x-direction, so it will not deflect particles with z but these particles also have x-components, we just don't know them."* It appears that this student is aware of the fact that "these particles also have x-components" but the student does not know how to find them. Many other students had similar difficulties on the pretest. Another difficulty students had with the orthogonality of states was mistakenly assuming that a spin-up state $|\uparrow\rangle_z$ is orthogonal to the spin-up state $|\uparrow\rangle_x$.

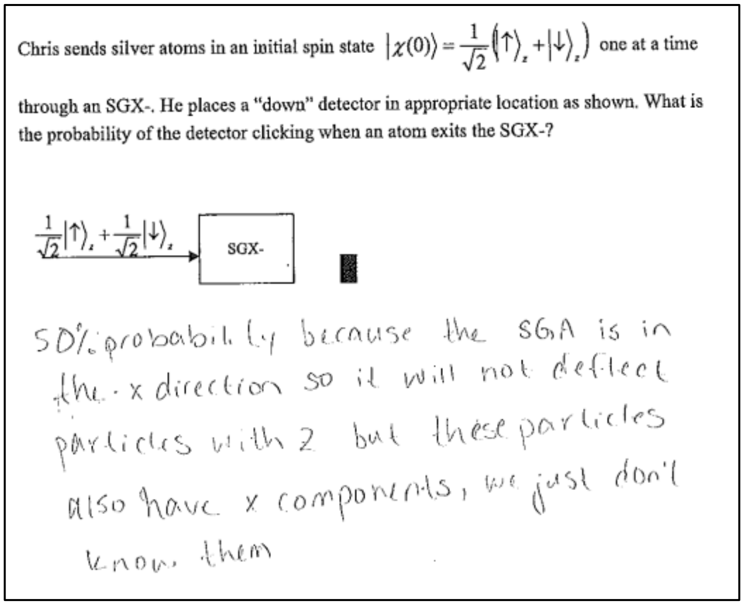

Figure 2.5 An example of a student response to Question 3 on test version A in which the student had difficulty recognizing that the initial state is an eigenstate of $\hat{S}_x$ so the entire beam will be deflected upward. The student states that the probability that the detector will click when an atom exits the SGX- is *"50% probability because the SGE is in the x-direction, so it will not deflect particles with z but these particles also have x-components, we just don't know them."*

Based on our results, the topic of different bases in question 3 on the pretest and posttest is an area in which the SGE MQS should be refined to improve student understanding. Moreover, Table 2.3 (see Appendix I) shows that students who obtained version A of the test as a pretest and version B of the test as a posttest showed moderate gains from the implementation of the SGE MQS, but the same did not hold true for those who obtained version B as a pretest and version A as a posttest (see Table 2.4 in Appendix I). Apart from differences between students and instructor implementation in two consecutive years (even though each instructor implemented them using similar approaches to the best of their abilities, there still may be individual differences), one issue that may contribute to the difference between question 3 performances of these two classes in Tables 2.3 and 2.4 is that students in Table 2.4 received this question as a multiple-choice question on version B on their pretest and as an open-ended version A on their posttest shown in Appendix

III. In Table 2.3, students had the reverse situation with regard to the versions. Tables 2.3 and 2.4 suggest that the class assessed using version B performed better on this question on the posttest. We also note that the differences in pretest averages before engaging with MQS can likely be due to differences in instructors' lecturing styles and differences between students in two consecutive years, something we do not have any control over. Therefore, we do not want to dwell on the pretest differences on any question in Tables 2.3 and 2.4. However, regardless of the pretest performance in Tables 2.3 and 2.4, the posttest performance on both versions of question 3 (see Tables 2.3 and 2.24 in Appendix I) after the SGE MQS shows room for improvement with regard to helping students learn to transform from one basis to another to analyze measurement outcomes after passing through a SGA with a particular magnetic field gradient. We are contemplating adding another question to provide additional coaching and scaffolding to students in order to solidify their conceptual understanding of how to transform from one basis to another depending upon the magnetic field grading in the Stern Gerlach apparatus and to help students reason about the outcomes of measurement after the atoms pass through a SGA.

Question 5 assesses student proficiency in differentiating between a mixture and superposition of states and showed weak improvement after implementation of the MQS (see Tables 2.1, 2.3 and 2.4). Even after engaging with the MQS, which strived to help students learn to differentiate between a superposition state, $|\chi\rangle = \sqrt{\frac{7}{10}}|\uparrow\rangle_z + \sqrt{\frac{3}{10}}|\downarrow\rangle_z$ and an analogous mixture made up of 70% $|\uparrow\rangle_z$ particles and 30% $|\downarrow\rangle_z$ particles, students struggled with this concept. Previously, students using the SGE QuILT had shown much stronger gains (Table 2.2). We are currently considering adding another multiple-choice question in the SGE MQS to have students further reflect upon the difference between a superposition of states and a mixture.

2.7 SUMMARY

Well-designed multiple-choice questions with peer discussions are excellent tools for engaging students in the learning process and relatively easy to implement in the classroom, with or without the use of clickers, compared to many other evidence-based active-engagement pedagogies. We describe a framework for developing and validating multiple-choice question sequences and the development, validation and in-class implementation of a MQS focusing on the fundamental concepts in quantum mechanics using the Stern-Gerlach experiment that was inspired by the learning objectives and guided learning sequences in the corresponding QuILT [66]. The SGE MQS was developed using research on student difficulties in learning these fundamental concepts of quantum mechanics as a guide. Different questions in the MQS build on each other and strive to help students organize, extend and repair their knowledge structure. One useful aspect of the Stern Gerlach experiment is that it can help students learn about foundational issues in quantum mechanics using a very simple two state model. In particular, the MQS focuses on helping students learn about important issues in quantum mechanics such as the difference between the Hilbert space and physical space, how to prepare a quantum state, how to analyze the outcomes of a particular set up involving various Stern-Gerlach devices and an initial spin state of neutral silver atoms, and the difference between a superposition state vs. a mixture (and how the SGAs with appropriate orientations of magnetic field gradients can be used to differentiate between these). This MQS is composed of seven questions most of which are posed in concrete contexts with different initial spin states of a beam of neutral silver atoms sent through various SGAs. Only the last question, which focuses on helping students differentiate between a superposition and mixture, concerns an abstract case in which students are asked for the outcome in a situation for which they must consider more than one possible setup to answer correctly. The entire MQS can be spread across separate lecture periods, or can be implemented together, e.g., to review the concepts.

Development of a research-validated learning tool such as the SGE MQS described here is an iterative process. After the in-class implementation of the SGE MQS using clickers and peer interaction by two different instructors, we found that the MQS was effective in helping students learn many of the important concepts. However, in-class evaluation also shows that further scaffolding is needed to guide students in differentiating between a quantum state which is a superposition of eigenstates of an operator corresponding to an observable from a mixture. Appropriate modifications are being made to the SGE MQS so that this issue can be addressed in the future iterations and implementations. Moreover, while both instructors implemented the MQS by interspersing them with lectures using clickers and peer interaction, future research can evaluate the effectiveness of these validated MQS in other modes of classroom implementations.

2.8 ACKNOWLEDGEMENTS

We thank the National Science Foundation for award PHY-1806691 as well as thank the faculty and students for help.

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2.10 CHAPTER APPENDIX

2.10.1 Individual class data

Table 2.3 Comparison of mean pre/posttest scores on each question, normalized gains and effect sizes for upper-level undergraduate students in QM who engaged with the SGE MQS when version A was used for pretest and version B was used for posttest (total number of students N = 17).

Question	Pretest Mean	Posttest Mean	Normalized Gain (g)	Effect Size (d)
1	38%	100%	1.00	1.05
2	14%	97%	0.97	1.79
3	41%	65%	0.40	0.24
4	38%	79%	0.67	0.51
5	12%	59%	0.53	0.64
6	41%	74%	0.55	0.34

Table 2.4 Comparison of mean pre/posttest scores on each question, normalized gains and effect sizes for upper-level undergraduate students in QM who engaged with the SGE MQS when version B was used for pretest and version A was used for posttest (total number of students N = 31).

Question	Pretest Mean	Posttest Mean	Normalized Gain (g)	Effect Size (d)
1	74%	93%	0.72	0.28
2	53%	89%	0.77	0.45
3	35%	41%	0.09	0.06
4	58%	80%	0.53	0.30
5	31%	43%	0.18	0.14
6	44%	88%	0.78	0.55

2.10.2 Additional MQS questions

(MQ3) *A beam of neutral silver atoms in a spin state* $|\chi\rangle = a|\uparrow\rangle_z + b|\downarrow\rangle_z$ *is sent through a SGX-. An "up" detector blocks some silver atoms, as shown in Figure 2.6. What fraction of the initial atoms will be blocked by the detector?*

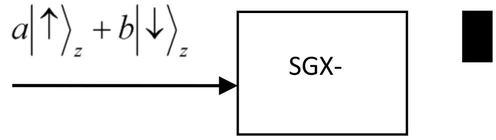

Figure 2.6 Figure for MQ3 using the representation as describeded in Figure 2.1.

a) $|a|^2$
b) $|b|^2$
c) $\boldsymbol{\frac{1}{2}|a+b|^2}$
d) $\frac{1}{2}|a-b|^2$
e) None of the above

(MQ4) *A beam of neutral silver atoms is in the initial spin state* $|\uparrow\rangle_z$*. It propagates through two SGAs as shown in Figure 5. What is the probability that detector B will click for the atoms that enter the first SGA?*

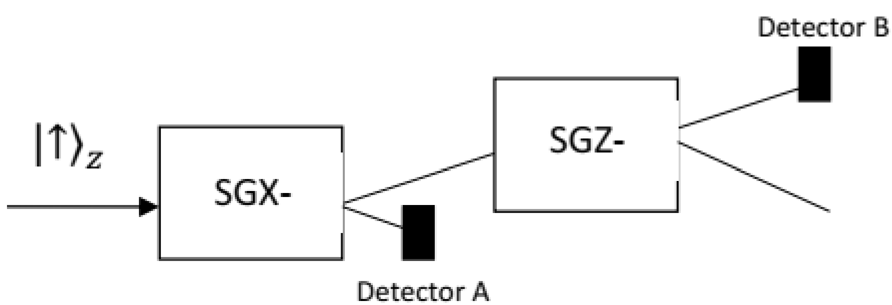

Figure 2.7 Figure for MQ4 using the representation as described in Figure 2.1.

a) $1/2$
b) $\boldsymbol{1/4}$
c) $1/8$
d) 1
e) None of the above

(MQ5) *The initial state of a beam of neutral silver atoms is $|\uparrow\rangle_z$. It propagates through three SGEs as shown in Figure 2.8. What is the probability that the detector will click for the atoms that enter the first SGE?*

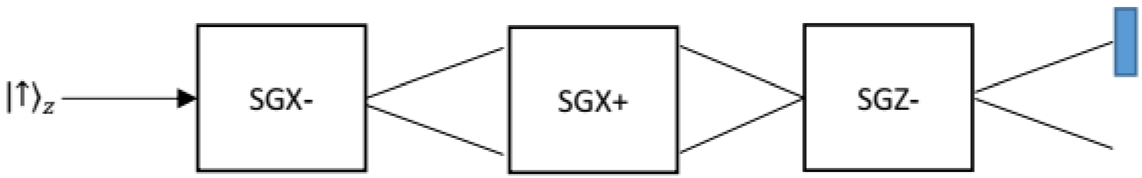

Figure 2.8 Figure for MQ5 using the representation as described in Figure 2.1.

a) $^1/_2$
b) $^1/_4$
c) $^1/_8$
***d)* 1**
e) None of the above

(MQ6) *The initial state of a beam of neutral silver atoms is $|\uparrow\rangle_z$. Suppose you want to prepare a beam of neutral silver atoms in spin state $|\downarrow\rangle_z$. Which of the options in Figure 2.9 shows an appropriate SGE to collect neutral silver atoms (not intercepted by a detector) in spin state $|\downarrow\rangle_z$?*

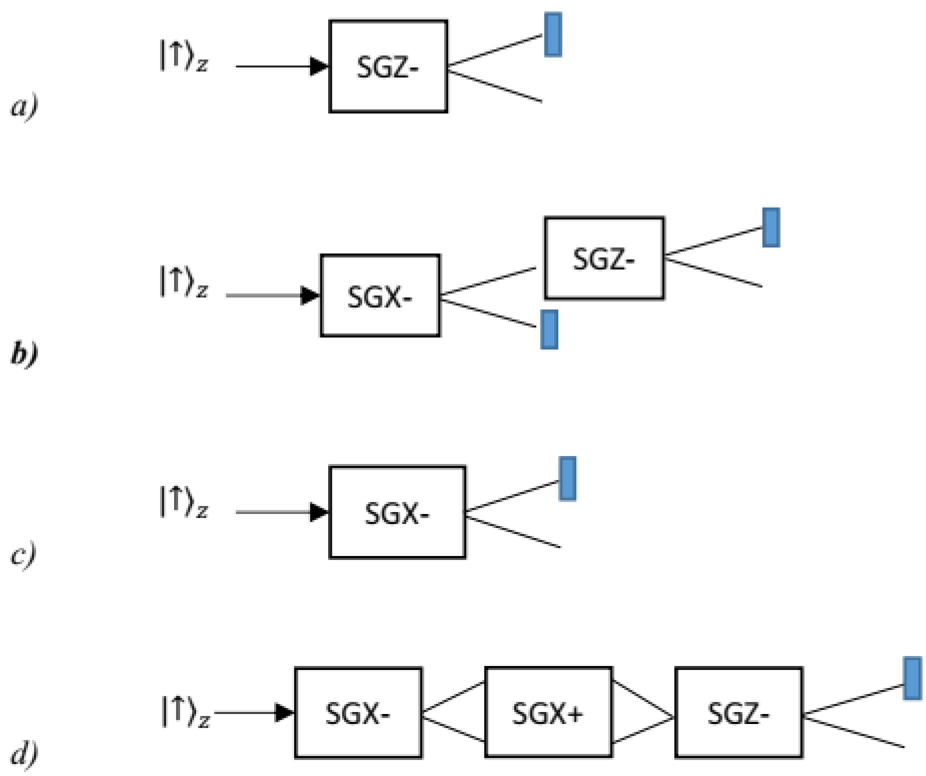

Figure 2.9 Figure for MQ6 using the representation as described in Figure 2.1.

(MQ7) *Suppose neutral silver atoms are in an unknown spin state. The spin state is either a mixture with 70% of the atoms in the* $|\uparrow\rangle_z$ *state and 30% in the* $|\downarrow\rangle_z$ *state or it is a superposition state* $|\chi\rangle = \sqrt{\frac{7}{10}}|\uparrow\rangle_z + \sqrt{\frac{3}{10}}|\downarrow\rangle_z$. *Choose all of the following states that are correct about the beam propagating through an SGZ or SGX apparatus:*

I. *When the beam propagates through the SGZ, 70% of the atoms will register in one detector and 30% of the atoms will register in the other, regardless of the two possibilities for the state.*
II. *When the beam propagates through the SGX, 50% of the atoms will register in one detector and 50% of the atoms will register in the other, regardless of the two possibilities for the state.*
III. *We can use a SGZ to distinguish between the possible spin states of the incoming silver atoms.*

a) I only
b) II only
c) III only
d) II and III only
e) None of the above

2.10.3 Additional test questions

3. (version B) Harry sends silver atoms all in the normalized spin state $|\chi(t=0)\rangle = a|\uparrow\rangle_z + b|\downarrow\rangle_z$ through a SGX-. He places an "up" detector as shown to block some silver atoms and collects the atoms coming out in the "lower channel" for a second experiment. What fraction of the initial silver atoms will be available for his second experiment? What is the spin state prepared for the second experiment? Show your work.

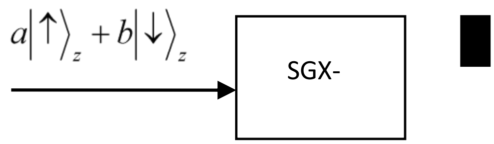

Figure 2.10 Figure for Question 3 on version B that focuses on the learning objective related to transforming the initial state to a basis that makes the analysis of measurement outcomes after passing through the SGA convenient (as well as on how to determine the spin state that is prepared and the fraction of the atoms that are in that final state prepared (i.e., not intercepted by the detector).

4. (version B) Sally sends silver atoms in state $|\uparrow\rangle_z$ through three SGAs as shown below. A detector is placed either in the up or down channel after each SGA as shown. Note that each SGA has its magnetic field gradient in a different direction. Next to each detector, write down the probability that the detector clicks. The probability for the clicking of a detector refers to the probability that a particle entering the **first** SGA reaches that detector. Also, after each SGA, write the spin state Sally has prepared. Explain.

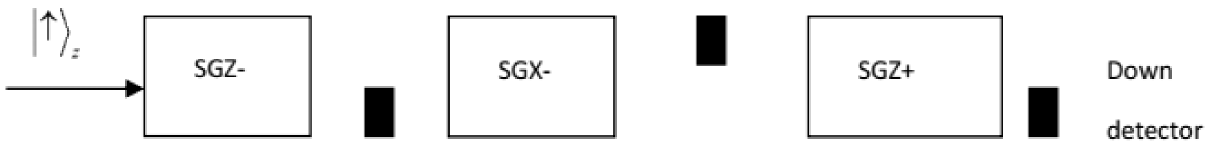

Figure 2.11 Figure for Question 4 on version B that corresponds to the learning objective related to preparing a final quantum state which is orthogonal to the initial state. On both versions of this test question, students were given an arrangement of Stern-Gerlach apparati and were asked to determine the probability that each detector clicks and the spin state prepared.

5 (version A) Suppose beam A consists of silver atoms in the state $|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_z + |\downarrow\rangle_z)$, and beam B consists of an unpolarized mixture in which half of the silver atoms are in state $|\uparrow\rangle_z$ and half are in state $|\downarrow\rangle_z$. Design an experiment with **SGA**s and **detectors** to differentiate these two beams. Sketch your experiment setup below and explain how it works.

5. (version B) Suppose beam A consists of silver atoms in the state $|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_z + |\downarrow\rangle_z)$, and beam B consists of an unpolarized mixture in which half of the silver atoms are in state $|\uparrow\rangle_z$ and half are in state $|\downarrow\rangle_z$. Choose all of the following statements that are correct.

(1) Beam A will not separate after passing through **SGZ-**.
(2) Beam B will split into two parts after passing through **SGZ-**.
(3) We can distinguish between beams A and B by passing each of them through a **SGX-**.

A. only 1
B. only 2
C. 1 and 2
D. ***2 and 3***
E. All of the above.

6. (version B) Suppose you have a beam of atoms in the spin state $|\chi(0)\rangle = |\downarrow\rangle_z$ but you need to prepare the spin state $|\uparrow\rangle_z$ for your experiment. Could you use SGAs and detectors to prepare the spin state $|\uparrow\rangle_z$? If yes, sketch your setup below and explain how it works. If no, explain why.

3.0 INSTRUCTIONAL PRAGMATISM: USING A VARIETY OF EVIDENCE-BASED APPROACHES FLEXIBLY TO IMPROVE STUDENT LEARNING

3.1 INTRODUCTION

3.1.1 Background

A major goal of many physics courses from introductory to advanced levels is to help students learn physics concepts [1-13] while also developing their problem solving and reasoning skills [14-28]. We have been studying how students in physics courses can learn to think like a physicist and develop a solid grasp of physics concepts [29-45]. Many researchers have been involved in developing and evaluating evidence-based active-engagement (EBAE) curricula and pedagogies [1-45] to improve student learning, but implementation of these EBAE approaches to help students learn has been slow. Some major barriers to implementation of the EBAE pedagogies at the college-level include lack of faculty buy-in and their reluctance and/or resistance, partly due to a lack of an institutional reward system for using these evidence-based approaches, the time commitment involved in effectively adapting and implementing them, and instructors' fear that their students may complain (since students may prefer to passively listen to lectures as opposed to actively engage in the learning process) [46]. Moreover, the amount of class time required to implement an EBAE pedagogy, the flexibility with which it can be implemented, the need to train instructors in how to effectively use it, and the architectural constraints of the classrooms may also increase the barrier and make it difficult to implement an EBAE pedagogy [46]. Because of this, even those instructors who adopt and adapt EBAE curricula and pedagogies in their classes are often disappointed when they do not observe the learning gains they expected and may quit employing the EBAE methods.

3.1.2 Instructional Pragmatism Framework

One major cause for the low *sustained* usage of the EBAE learning tools and pedagogies among the adopters is that the early adaptations in their classes do not necessarily show the same large gains in student learning as those observed by their developers [46]. One reason for this failure to replicate the positive outcomes of an innovation in early implementations by instructors is that the EBAE approaches must be refined and tweaked to suit the instructor's style and their students' prior knowledge and skills as well as their motivational characteristics. Also, the bandwidth for the different ways in which EBAE curricula and pedagogies can be adapted, implemented and still be successful in producing desired student learning is limited. Thus, if an EBAE curriculum or pedagogy is replicated in a somewhat modified form and does not produce the desired learning outcome, instructors may feel disappointed and quit using that innovative EBAE approach. Instructional pragmatism framework advocates that when an EBAE approach does not appear to be successful in improving student learning, instructors should be flexible and persistent and remind themselves that improving teaching and learning is a process that requires refinement and tweaking to yield desired outcome. Therefore, instead of giving up on the EBAE approaches, they should cultivate instructional pragmatism, keep several EBAE approaches in their tool box and be pragmatic about adopting and adapting various EBAE approaches that meet the needs of their students as well as the constraints of their classroom in order to help their students master physics concepts.

3.1.3 Goal and motivation

The goal and motivation of this work are to illustrate an example of instructional pragmatism in which a quantum physics instructor did not lose hope when an EBAE method involving implementation of a sequence of clicker questions on addition of angular momentum did not yield expected learning outcomes on the posttest administered after the clicker question sequence even though it was found effective in earlier implementations by other instructors. Instead, the instructor viewed improving teaching and learning as a continuous process, remained optimistic and employed another EBAE method with the same set of students and implemented it as homework that did not require him to spend more time in class on this topic. In particular, the instructor created an out of class opportunity for students to productively struggle [47-49] with the same posttest problems on addition of angular momentum that they had not performed well on by incentivizing them to correct their mistakes before providing the correct solution. The instructor's flexibility and use of another field-tested pedagogy, "incentives for learning from mistakes," appear to be effective in that students' performance on one of the addition of angular momentum problems posed on the final exam shows that students who corrected their mistakes benefited from the exercise and learned about addition of angular momentum better than those who did not correct their mistakes. We argue that supporting and aiding physics instructors to embrace instructional pragmatism can go a long way in helping their students learn physics since it will encourage them to be persistent in using various EBAE approaches flexibly as they refine and tweak their implementation.

3.1.4 Background on clicker questions

Here we discuss instructional pragmatism in the context of a quantum mechanics course in which instructors first used an EBAE pedagogy involving sequences of clicker questions. Clicker questions (also known as concept tests) are conceptual multiple-choice questions typically administered in the classroom to engage students in the learning process and obtain feedback about their learning via a live feedback system called clickers [50-56]. Integration of peer interaction with lectures via clicker questions has been popularized in the physics community by Mazur [50]. In Mazur's approach, the instructor poses conceptual, multiple-choice clicker questions to students which are interspersed throughout the lecture. Students first answer each clicker question individually, which requires them to take a stand regarding their thoughts about the concept(s) involved. Students then discuss their answers to the questions with their peers and learn by articulating their thought processes and assimilating their thoughts with those of the peers. Then after the peer discussion, they answer the question again using clickers, followed by a general class discussion about those concepts in which both students and the instructor participate. The feedback that the instructor obtains is also valuable because it provides an estimate of the prevalence of student common difficulties and the fraction of the class that has understood the concepts and can apply them in the contexts in which the clicker questions are posed. The use of clickers keeps students alert during lectures and helps them monitor their learning. Clicker questions can be used in the classroom in different situations, e.g., they can be interspersed within lectures to evaluate student learning in each segment of a class focusing on a concept, at the end of a class or to review materials from previous classes at the beginning of a class. While clicker questions for introductory [50-56] and upper-level physics such as quantum mechanics [57] have been developed, there have been very few documented efforts [58] toward a systematic development and validation of clicker question sequences (CQSs), e.g., question sequences on a given concept that can be used in a few class periods when students learn the concepts and that build on each other effectively to help students organize their knowledge structure.

3.1.5 Background on "Incentives for Learning from Mistakes" pedagogy

The discussion of instructional pragmatism in the context of a quantum mechanics course here involves an instructor using an EBAE pedagogy that involves giving incentives to students to learn from their mistakes when the CQS did not yield the desired outcome on the posttest after CQS implementation. In order to appreciate the ILM pedagogy, we must recognize that two characteristics of physics experts are that they have learned how to learn and they use problem solving as an opportunity for learning [59-63]. In particular, experts automatically reflect upon their mistakes in their problem solution in order to repair, extend and organize their knowledge structure. Unfortunately, for many students, problem solving is a missed learning opportunity [59,60]. Without guidance, students often do not reflect upon the problem solving process after solving problems in order to learn from them nor do they make an effort to learn from their mistakes after the graded problems are returned to them [59,60]. The incentives for learning from mistakes pedagogy are based on the tenet that instructors can explicitly prompt students to learn from their mistakes by rewarding them for correcting their mistakes [61-63]. This type of activity over time can also help them learn to make use of problem solving as a learning opportunity.

Here we discuss instructional pragmatism in the context of implementation of ILM pedagogy in a junior/senior level quantum mechanics course when a CQS did not yield the learning gains expected by the instructor. Prior research has focused on how introductory physics students differ from physics experts and strategies that may help introductory students learn to learn [61-

62]. By comparison, few investigations have focused on the learning skills of advanced physics students [63], although investigations have been carried out on the difficulties advanced students have with various advanced topics such as quantum physics [64-107]. In fact, it is commonly assumed that most physics majors in junior and senior years have not only learned a wide body of physics content but have also picked up the habits of mind and self-monitoring skills needed to build a robust knowledge structure [63]. Many physics instructors take for granted that advanced physics students will learn from their own mistakes in problem solving without explicit prompting, especially if students are given access to clear solutions. It is implicitly assumed that, unlike introductory students, advanced students have become independent learners and will take the time out to learn from their mistakes, even if the instructors do not reward them for fixing their mistakes, e.g., by explicitly asking them to turn in, for course credit, a summary of the mistakes they made and writing down how those mistakes can be corrected [63]. However, such assumptions about advanced students' superior learning and self-monitoring skills have not been substantiated by research. In an earlier investigation, Mason and Singh [60] investigated the extent to which upper-level students in quantum mechanics learn from their mistakes. They administered four problems in the same semester twice, both on the midterm and final exams in an upper-level quantum mechanics course. The performance on the final exam shows that while some students performed equally well or improved compared to their performance on the midterm exam on a given question, a comparable number performed poorly both times or regressed (i.e., performed well on the midterm exam but performed poorly on the final exam). The wide distribution of students' performance on problems administered a second time points to the fact that many advanced students may not automatically exploit their mistakes as an opportunity for repairing, extending, and organizing their knowledge structure. Mason and Singh also conducted individual interviews with a subset of students to delve deeper into students' attitudes toward learning and the importance of organizing knowledge. They found that many students focused on selectively studying for the exams and did not necessarily look at the solutions provided by the instructor for the midterm exams to learn, partly because they did not expect those problems to be repeated on the final exam and/or found it painful to confront their mistakes.

The ILM pedagogy proposes giving incentives to students for learning from their mistakes, e.g., by explicitly rewarding them for correcting their mistakes before giving them the correct solutions because productive struggle while diagnosing one’s mistakes and learning from them can be an excellent learning opportunity both for learning content and developing useful skills. Students may gain a new perspective on their mistakes by asking themselves reflective questions while solving the problems correctly making use of the resources, e.g., their class notes and textbook available to them. In a prior study spanning four years in which advanced undergraduate physics students taking a quantum mechanics course, these students were given the same four problems in both the midterm exam and final exam (similar to the Mason and Singh study [63]). Approximately half of the students were given incentives to correct their mistakes in the midterm exam and could get back up to 50% of the points lost on each midterm exam problem. The solutions to the midterm exam problems were provided to all students but those who corrected their mistakes were provided the solution *after* they submitted their corrections to the instructor. The performance on the final exam on the same problems suggests that students who were given incentives to correct their mistakes significantly outperformed those who were not given an incentive [63]. It was found that the incentive to correct the mistakes on the midterm exam had the greatest impact on the final exam performance of students who did poorly on the midterm exam, which is very encouraging [63].

3.1.6 Organization of chapter

The rest of the chapter is organized as follows. Since CQS was used as the first EBAE pedagogy by the instructors, in section II, we discuss the learning goals and methodology for the development, validation and in-class implementation of the clicker question sequence on addition of angular momentum. In section III, we discuss a case in which the implementation of the CQS did not produce the desired performance on the posttest. The instructor subsequently used another EBAE pedagody, which offered grade incentive to the students for correcting their own mistakes. In section IV, we conclude with a discussion and summary.

3.2 THE EBAE APPROACH INVOLVING CLICKER QUESTIONS SEQUENCE

Before we discuss how the CQS on addition of angular momentum in quantum mechanics (QM) was implemented by the instructors, we summarize its development and validation process including its learning goals. This CQS was developed for students in upper-level undergraduate QM courses by taking advantage of the learning goals and inquiry-based guided learning sequences in a research-validated Quantum Interactive Learning Tutorial (QuILT) on this topic [105,106] as well as by refining, fine-tuning and adding to the existing clicker questions from our group which have already been individually validated [107]. The CQS can be used in class either separately from the QuILT or synergistically with the corresponding QuILT [105] if students engage with the QuILT after the CQS as another opportunity to reinforce the concepts learned.

The learning goals and inquiry-based learning sequences in the QuILT, which guided the development and sequencing of the CQS questions, were developed using extensive research on student difficulties with these concepts as a guide and cognitive task analysis from an expert perspective.

3.2.1 Learning Goals

One learning goal of the CQS (consistent with the QuILT) is that students should be able to identify the dimensionality of the product space of the spin of two particles. For example, if a system consists of two spin-1 particles with individual three-dimensional spin Hilbert spaces, the product space of the two spin system is the product of those dimensions, 3×3=9 (not the sum of dimensions, 3+3=6). Another learning goal of the CQS is that students are able to choose a suitable representation, such as the "uncoupled" or "coupled" representation, and construct a complete set of basis states for the product space in that representation. We note that the concepts related to the addition of orbital and spin angular momenta are analogous so here we will only focus on spin. In standard notation, the basis states in the uncoupled representation are eigenstates of $\hat{S}_1^2$, $\hat{S}_{z1}$, $\hat{S}_2^2$ and $\hat{S}_{z2}$ and can be written as $|s_1, m_{s1}\rangle \otimes |s_2, m_{s2}\rangle$. Here each particle's individual spin and z-component of spin quantum numbers are s_1, s_2 and m_{s1}, m_{s2}, respectively. On the other hand, in the coupled representation, the basis states, $|s, m_s\rangle$, are eigenstates of $\hat{S}_1^2$, $\hat{S}_2^2$, $\hat{S}^2$, and $\hat{S}_z$ where $\hat{\vec{S}} = \hat{\vec{S}}_1 + \hat{\vec{S}}_2$ and the total spin quantum number, s, and the z-component of the spin quantum number, m_s, are for the entire system. Students should be able to use the addition of angular momentum to determine that the total spin quantum number of the system s can range from $s_1 + s_2$ down to $|s_1 - s_2|$, with integer steps in between, where s_1 and s_2 are the individual spin quantum numbers for the particles. The z-component of the spin of the composite system is $m_s = m_{s1} + m_{s2}$. Another learning goal of the CQS is that students be able to calculate matrix elements of various operators corresponding to observables (e.g., a Hamiltonian in the product space) in different representations.

3.2.2 Development and Validation

Based upon the learning goals of the QuILT, questions in the addition of angular momentum CQS were developed or adapted from prior validated clicker questions and sequenced to balance difficulties, avoid change of both concept and context between adjacent questions as appropriate in order to avoid cognitive overload [108], and include a mix of abstract and concrete questions to help students develop a good grasp of the concepts. The validation was an iterative process.

After the initial development of the addition of angular momentum CQS using the learning goals and inquiry-based guided sequences in the QuILT and existing individually validated CQSs, we iterated the CQS with three physics faculty members who provided valuable feedback on fine-tuning and refining both the CQS as a whole and some new questions that were developed and adapted with existing ones to build the CQS to ensure that the questions were unambiguously worded and build on each other based upon the learning goals. We then conducted individual think-aloud interviews with advanced students who had learned these concepts via traditional lecture-based instruction in relevant concepts to ensure that they interpreted the CQS questions as intended and the sequencing of the questions provided the appropriate scaffolding support to students. This version of the CQS has 11 questions, which can be grouped into three sections (to be discussed below) and can be integrated with lectures in which these relevant concepts are covered in a variety of ways based upon the instructor's preferences.

The addition of angular momentum CQS has three sections that can be used separately or together depending, e.g., upon whether these are integrated with lectures similar to Mazur's approach, used at the end of each class or used to review concepts after students have learned via lectures everything related to addition of angular momentum that the instructor wanted to teach. The first section of the CQS, CQ1-CQ3, focuses on the uncoupled representation with basis states $|s_1 m_{s1}\rangle \otimes |s_2, m_{s2}\rangle$. The first question focuses on student understanding of the notation for the basis states in this representation along with the dimensionality of the product space and be able to write a complete set of basis states looks like. Following this question, CQ2 and CQ3 build on this understanding, asking students to identify the operators for which the basis states in the uncoupled representation are eigenstates and about some diagonal and off-diagonal matrix elements of various operators and whether they are zero or non-zero (i.e., determining whether operators are diagonal in the uncoupled representation). This section of the CQS concludes with a class discussion in which the instructor may review characteristics of this representation, as well as address any common difficulties exhibited by students.

The second section of this CQS, CQ4-CQ6, deals with the coupled representation with basis states $|s, m_s\rangle$ (where s_1 and s_2 are suppressed). The structure and concepts in these questions shown below are analogous to the structure of the first section, allowing students to compare and contrast these two representations.

(CQ4) *Choose all of the following statements about the product space for a system of* ***two spin-1/2 particles*** *in the* ***coupled representation*** *that are correct:*

I. *The dimensionality of the product space is the product of the dimensions of each particle's* *subspace, which is 2x2=4.*

II. $|s,\ m_s\rangle$ *is an appropriate form for the basis states, where s ranges from* $|s_1$-$s_2|$ *to* s_1+s_2 *by integer steps, and* m_s=m_{s1}+m_{s2}, *ranging from –s to s in integer steps for each s.*

III. $|1,1\rangle$, $|1,0\rangle$, $|1,-1\rangle$, *and* $|0,0\rangle$ *are the elements of a complete set of basis states.*

a) I only

b) b) I and II only

c) c) I and III only

d) II and III only

e) All of the above

(CQ5) *Choose all of the following statements about the product space for a system of* ***two spin-1/2 particles*** *in the* ***coupled representation*** *that are correct:*

I. *Basis state* $|1,-1\rangle$ *is an eigenstate of* $\hat{S}^2$ *such that* $\hat{S}^2|1,-1\rangle = 2\hbar^2|1,-1\rangle$.

II. *Basis state* $|1,-1\rangle$ *is an eigenstate of both* $\hat{S}_1^2$ *and* $\hat{S}_2^2$ *such that* $\hat{S}_1^2|1,-1\rangle = 2\hbar^2|1,-1\rangle$ *and* $\hat{S}_2^2|1,-1\rangle = 2\hbar^2|1,-1\rangle$.

III. *Basis state*$|1,-1\rangle$ *is an eigenstate of* $\hat{S}_{z1}$, $\hat{S}_{z2}$, *and* $\hat{S}_z$.

a) I only

b) I and II only

c) I and III only

d) II and III only

e) All of the above

(CQ6) *Consider the product space of a system of* ***two spin-1/2 particles****. Choose all of the following that are correct regarding the scalar products in the coupled representation. (Recall that these scalar products give the matrix elements of the* $\hat{S}_{1z} + \hat{S}_{2z}$ *operator in this basis).*

I. $\langle 1,1|(\hat{S}_{z1} + \hat{S}_{z2})|1,0\rangle = \langle 1,1|\hat{S}_z|1,0\rangle = 0$

II. $\langle 1,-1|(\hat{S}_{z1} + \hat{S}_{z2})|1,-1\rangle = \langle 1,-1|\hat{S}_z|1,-1\rangle = -\hbar$

III. $(\hat{S}_{z1} + \hat{S}_{z2})$ *is diagonal in the coupled representation.*

IV. $(\hat{S}_{z1} + \hat{S}_{z2})$ *is diagonal in the uncoupled representation.*

a) II and III only

b) I, II, and III only

c) I and IV only

d) I, II, and IV only

e) All of the above.

As noted, the first two sections of the addition of angular momentum CQS deal with only one representation at a time, and only with a system of two spin-1/2 particles. This choice is deliberate by design to avoid cognitive overload and allow students to revisit these representations in a familiar context since typical instruction on these concepts tends to emphasize a system of two spin-1/2 particles first.

The third section of the CQS extends these concepts to higher dimensional product spaces for both coupled and uncoupled representations. For example, CQ7 deals with the dimensionalities of the product space for systems of two spins that are not both spin-1/2. Then, CQ8 and CQ9 ask students to identify basis states in the coupled and uncoupled representations for these less familiar two-spin systems. Also, CQ12 and CQ13 ask students to identify the basis in the product space in which given Hamiltonians are diagonal (note that these are numbered differently because two questions were added after CQ9 later on). These Hamiltonians are comprised of operators addressed previously in the first questions of the CQS.

3.2.3 In-class implementation by instructor A

A The CQS was implemented with peer discussion [50] in an upper-level undergraduate QM class at a large research university (Pitt) after traditional lecture-based instruction in relevant concepts on the addition of angular momentum in which students learned about the coupled and uncoupled representations not only for a system of two spin-1/2 particles but also for systems for which the product spaces involve higher dimensions. Prior to the implementation of the CQS in class, students took a pretest after traditional instruction in each class, which was developed and validated by Zhu et al. [105] to measure comprehension of the concepts of addition of angular momentum. The first six questions in the CQS were implemented together right after the pretest. The last five questions in the third section of the addition of angular momentum CQS were implemented at the beginning of the next class to review concepts covered earlier in the lectures on product spaces involving higher dimensions. The posttest was administered during the following week to measure the impact of the CQS.

On the pretest, students were given a system of two spin-1/2 particles and a spin-spin interaction Hamiltonian, $\hat{\mathrm{H}}_1 = \left({}^{4E_0}/_{\hbar^2}\right)\hat{\mathrm{S}}_1 \cdot \hat{\mathrm{S}}_2 \ = \left({}^{2E_0}/_{\hbar^2}\right)(\hat{\mathrm{S}}^2 - \hat{\mathrm{S}}_1^2 - \hat{\mathrm{S}}_2^2)$, and a magnetic field-spin interaction Hamiltonian, $\hat{\mathrm{H}}_2 = -\mu\mathrm{B}\left(\hat{S}_{z1} + \hat{S}_{z2}\right)$, and asked to answer these questions:

(a) *Write down a complete set of basis states for the product space of a system of two spin-1/2 particles. Explain the labels you are using to identify your basis states.*

(b) *Evaluate one diagonal and one off-diagonal matrix element of the Hamiltonian $\hat{H}_1$ (of your choosing) in the basis you have chosen. Label the matrix elements so that it is clear which matrix elements they are.*

(c) *Evaluate one diagonal and one off-diagonal matrix element of the Hamiltonian $\hat{H}_2$ (of your choosing) in the basis you have chosen. Label the matrix elements so that it is clear which matrix elements they are.*

(d) *Are both Hamiltonians $\hat{H}_1$ and $\hat{H}_2$ diagonal matrices in the basis you chose*?

The posttest that students were administered following the implementation of the CQS was analogous to the pretest [5] and asked the same questions as the pretest but for a system of one spin-1/2 particle and one spin-1 particle. These pre/posttests are very similar to those administered by Zhu et al. to measure student learning after traditional instruction and after engaging with the addition of angular momentum QuILT [105]. However, due to time constraints in the classroom, questions (b) and (c), which had previously asked students to construct the entire matrix representation of the Hamiltonians, were reduced as stated earlier to evaluation of only one diagonal and off-diagonal matrix element [105]. In order to compare the performance of CQS and QuILT groups on pre/posttests so that the relative improvements can be determined, the same rubric was used for pre-/posttests given to the CQS students as the QuILT students in Ref. [105] (who were also advanced undergraduate students in QM). Questions (a), (b), and (c) were each worth 3 points, and students were awarded partial credit if only some basis states in (a) or some matrix elements in (b) or (c) were correct. Question (d) was worth 1 point (correct answer "yes or no").

3.2.4 In-class implementation results for CQS by instructor A in class A

Tables 3.1 and 3.2 compare pre/posttest performances of upper-level QM students from the same university in two different years after traditional lecture-based instruction (pretest) and on posttest after students had engaged with the CQS (Table 3.1) or QuILT (Table 3.2) on the addition of angular momentum. The normalized gain (or gain) is calculated as $g = (post\% - pre\%)/(100\% - pre\%)$ [2] and presented in both Tables 3.1 and 3.2 but effect size is calculated only in Table 3.1 (not available for Table 3.2 data in Ref. [105]). Effect size was calculated as Cohen's $d = (\mu_{post} - \mu_{pre})/\sigma_{pooled}$ where μ_i is the mean of group i and σ_{pooled} is the pooled standard deviation [109].

Table 3.1 Comparison of mean pre/posttest scores on each question, normalized gains and effect sizes for upper-level undergraduate QM students in class A who engaged with the CQS on addition of angular momentum concepts (N=16).

Question	Pretest Mean	Posttest Mean	Normalized Gain (g)	Effect Size (d)
(a)	59%	95%	0.88	0.30
(b)	24%	48%	0.31	0.22
(c)	17%	71%	0.66	0.44
(d)	14%	43%	0.33	0.67
Total	31%	69%	0.54	0.35

Table 3.2 Comparison of mean pre/posttest scores on each question and normalized gains from Ref. [105] (effect sizes not available) for upper-level undergraduate QM students who engaged with the QuILT on addition of angular momentum concepts (N=26).

Question	Pretest Mean	Posttest Mean	Normalized Gain (g)
(a)	77%	85%	0.35
(b)	8%	54%	0.50
(c)	8%	73%	0.71
(d)	31%	85%	0.78
Total	34%	72%	0.58

Although the number of students in each class is small and the pretest scores in Tables 3.1 and 3.2 are often different, they are low in both tables (except for question (a) in Table 3.2). However, the comparison of the posttest scores of the CQS group and the QuILT group in Tables 3.1 and 3.2 suggests that the CQS is effective in helping students learn to construct a complete set of basis states (question (a)) and calculate matrix elements for the magnetic field-spin interaction Hamiltonian (question (c)), garnering similar posttest scores to those of students who engaged with the QuILT. However, Table 3.1 also shows that students did not perform well on questions (b) and (d) even after engaging with the CQS. Review of student responses suggests that a major reason for the poor performance on both of these questions, even after the CQS, is due to the fact that a majority of students chose the basis to be the uncoupled representation (since it is the simpler representation for constructing the basis states) and then had difficulty with the matrix elements of the spin-spin interaction Hamiltonian in questions (b) and (d) since it is only diagonal in the coupled representation. In particular, in question (a), many students correctly constructed a complete set of basis states, but chose the uncoupled representation.

We note that while the magnetic field-spin interaction Hamiltonian in question (c) is diagonal in both coupled and uncoupled representations, calculating the matrix elements of the spin-spin interaction Hamiltonian in question (b) in the uncoupled representation is challenging since that operator is not diagonal in this basis. Along with a reasonable posttest score for question (a), the CQS group students' poor posttest score on questions (b) and (d) in Table 3.1 is due to the fact that while students learned to construct a complete set of basis states, many were not versed in calculating the matrix elements of an operator in a representation in which it is not diagonal as in question (b) (many students assumed that the spin-spin Hamiltonian in question (b) is also diagonal in the uncoupled representation, which it is not).

In fact, for question (d), even after the CQS, many students claimed that both Hamiltonians are diagonal in the uncoupled representation they had chosen. Since students were only asked to calculate a single off-diagonal matrix element in question (b), some students who correctly calculated an off-diagonal matrix element in question (b) that was zero concluded that the entire $\hat{H}_1$ matrix is diagonal in the uncoupled representation which it is not. On the other hand, a comparison of student performances on posttest in Tables 3.1 and 3.2 for questions (b) and (d) suggests that most students who engaged with the QuILT answered question (d) correctly but struggled to calculate matrix elements on the posttest in question (b).

Moreover, based on think-aloud interviews, we find that QM experts are more likely to consider whether different operators are diagonal in a given representation *before* choosing a basis to evaluate the matrix elements of the two Hamiltonians. They generally preferred to use the coupled representation since both Hamiltonians are diagonal in that representation (all off-diagonal matrix elements in questions (b) and (c) are zero). Since think-aloud interviews suggest that students did not, in general, automatically do this type of metacognition before selecting a basis for evaluating the matrix elements, the CQS was revised to explicitly offer such opportunity to students. In particular, more scaffolding was provided to help students construct a set of basis states that is not only complete, but is also convenient for evaluating the matrix elements of operators corresponding to the observables of interest (e.g., choosing the coupled representation would have made both Hamiltonians diagonal in the basis and made it significantly easier to calculate the matrix elements). We refined the second section of the CQS, which deals with the coupled representation, to offer additional practice in constructing a basis in this less familiar case. Also, the third section of the CQS was refined to offer more practice in identifying a representation in which a given operator is diagonal.

3.3 INSTRUCTIONAL PRAGMATISM: COMBINING TWO EBAE METHODS DYNAMICALLY

Before Instructional pragmatism which involves staying optimistic and persistent and continually refining an EBAE approach or changing to a different one and adapting it to fit the needs of their students dynamically is an invaluable skill for any instructor. While EBAE strategies are likely to provide promising results in a classroom after a few implementations, the instructors must consider the improvement in teaching and learning to be a process that may not yield the desired outcome in the first few implementations. In particular, the implementation of the EBAE methods needs to be refined and tweaked to suit instructors' teaching style and their students' prior knowledge and skills and is not a one-size-fits-all panacea. For this reason, it is important for instructors to have several EBAE instructional tools in their toolbox.

Following the implementation of the CQS in class A, which yielded reasonably good performance on two posttest questions but not on the other two posttest questions after students engaged with the CQS, two more clicker questions were developed and validated based upon the difficulties found after implementation in class A. These two new questions, CQ10 and CQ11, along with guided discussion after existing CQ12 and CQ13 (see the Appendix), were added to provide more support for addressing difficulties with working in the coupled representation and identifying convenient bases for answering different questions. This slightly amended CQS was then implemented in class B by instructor B, who was a different instructor than that for class A. The implementation of the CQS in class B followed the same procedure discussed in the preceding section for class A.

Table 3.3 shows class B's performance on all parts of both the pretest and posttest. Table 3.3 shows that students' average posttest performance was poor except on question (a). They performed significantly worse than class A (in Table 3.1) even on question (c). Although the normalized gains and effect sizes on all questions are reasonable (see Table 3.3), the instructor of course B was concerned about the learning as measured by the posttest scores and the fact that a majority of students had not mastered the concepts. Although how the CQS was implemented in class B could have play an important role in why the students did not benefit significantly from it, one likely reason for not benefiting from the CQS is that students did not have sufficient initial knowledge (as evidenced by the pretest scores) before they engaged with the CQS. For example, when roughly half of the students know the correct answers to the clicker questions, the peer discussions during the implementation of the clicker questions is generally effective [50]. One possible reason for the low prior preparation as evidenced by the pretest scores may be that the instructor of class B did not spend sufficient time before the CQS on discussing the relevant underlying concepts (e.g., on questions (b) and (d), students in class B performed very poorly on the pretest as shown in Table 3.3 and for those questions their posttest scores are also less than 40%).

Table 3.3 Comparison of mean pre/posttest scores on each question, normalized gains and effect sizes for upper-level undergraduate QM students in class B who engaged with the CQS on addition of angular momentum concepts (N=19).

Part	Pretest Mean	Posttest Mean	Normalized Gain (g)	Effect Size (d)
(a)	46%	86%	0.74	0.26
(b)	5%	39%	0.35	0.30
(c)	12%	53%	0.46	0.30
(d)	3%	34%	0.32	0.66
Total	19%	57%	0.46	0.30

Following these posttest results on addition of angular momentum, the instructor used instructional pragmatism and implemented another active learning pedagogy. In particular, the instructor use the ILM pedagogy and returned the posttests to students with grades and incorrect parts marked but without explanations, and asked them to correct their mistakes as homework in return for up to half of the quiz points they had lost. Unlike the earlier implementation of the ILM pedagogy in quantum mechanics in which students were asked to correct their mistakes on midterm exam with similar incentives to earn 50% of the missed points (in which case all students corrected their mistakes), not all students took advantage of the opportunity because the posttest was a low stakes quiz worth less than 1% of a student's final grade in the course. Table 3.4 shows the results after 12 of the 19 students made corrections to their posttests. With instructional pragmatism and implementation of both the CQS and learning from mistakes pedagogies, students in class B who corrected their mistakes demonstrated better performance (see Table 3.4). Moreover, we note that instructor B gave question (c) as part of the midterm exam. After corrections, students who corrected their mistakes on the posttest obtained an average score of 85% on this problem. Meanwhile, students who did not correct their posttest obtained an average score of 71% (note that those who corrected their mistakes initially had a slightly lower score on this question than those who did not correct their mistakes). While students who did not correct their mistakes also performed better on the midterm exam (71%) since they also had access to the correct solution and had further opportunity to learn concepts, those who corrected their mistakes performed significantly better than them (85%).

Table 3.4 Comparison of mean score on each question before and after student corrections for upper-level undergraduate QM students in class B who engaged with the CQS on addition of angular momentum concepts and also engaged with the ILM pedagogy to learn from their mistakes. Columns showing only students who made corrections (N=12) are shown alongside the class average (N=19).

Part	**Initial Posttest**			**After Corrections**
	Correctors (N=12)	Non-Correctors (N=7)	All Participants (N=19)	Correctors (N=12)
(a)	94%	71%	86%	100%
(b)	47%	24%	39%	94%
(c)	50%	57%	53%	86%
(d)	25%	50%	34%	67%
Total	60%	51%	57%	91%

3.4 DISCUSSION AND SUMMARY

Physics education researchers have developed many evidence-based active engagement (EBAE) curricula and pedagogies and documented their effectiveness in certain physics classes at some institutions. While there are intense efforts being made to disseminate these EBAE curricula and pedagogies, their sustained adoption and adaptation in physics classes have been slow. Even instructors who adapt EBAE approaches in their classes often give up if they do not yield desirable learning outcomes in early implementation. Here we argue that physics instructors should be pragmatic about their instructional approaches and view improvement in their teaching and learning as a process. Instructional pragmatism also focuses on encouraging and supporting instructors to keep several EBAE learning tools and pedagogies in their toolbox. With the goal of improving their teaching and student learning, instructors should remain optimistic and flexible, dynamically combining various EBAE approaches if the results from the implementation of one of these EBAE approaches does not yield the desired outcome. Instructors should realize that all EBAE approaches have certain bandwidth of implementation in which they will be effective. Ensuring that the chosen approach is well-matched with their style and their students' prior knowledge and skills may take time. In particular, because different instructors have different teaching styles, and varying degrees of familiarity with the tools they are using, some tools may prove to be less effective than anticipated based on those reported in publications at least in earlier implementation so that an iterative approach with successive refinements will get them closer to their goal. Moreover, when an approach does not yield the desired learning outcome, an instructor should be pragmatic and be willing to improvise using additional EBAE methods commensurate with the constraints of their course in order to improve learning of students who did not benefit from one strategy.

We presented an example of instructor B with instructional pragmatism who first used clicker question sequences on addition of angular momentum because engaging students with well-designed clicker questions is one of the commonly used EBAE strategy in physics courses with a relatively low barrier to implementation. The in-class evaluation of the CQS using peer instruction in upper-level QM involved comparing students' performance after engaging with the CQS with previously published data from the QuILT pertaining to these concepts. This CQS was implemented by two instructors (A and B) in two QM classes in consecutive years. After the in-class implementation of the CQS on the addition of angular momentum in Class A, it was found that the CQS was effective in helping students construct a complete set of basis states in a product space and in calculating matrix elements for an operator that is diagonal in that basis. However, in-class evaluation also showed that a few additional questions can be included to guide students in selecting a representation that simplifies the task of calculating the matrix elements of an operator corresponding to an observable (e.g., choosing a basis in which the Hamiltonian operator is diagonal). Instructor A did not use additional EBAE methods to help students learn about these topics. The slightly modified CQS was then implemented the following year at the same institution by instructor B in QM Class B and student performance on many of the questions was worse than those of instructor A's students suggesting insufficient mastery of the concepts even after the CQS implementation.

As noted, this is not an uncommon occurrence for instructors adopting new instructional tools, as the instructional tool must be adapted to the instructor's style as well as students' prior preparation. In this case, because both before and after the CQS implementation, class B's conceptual understanding was lagging relative to both Class A and the QuILT group, instructor B adapted to his class's needs for further support. He pragmatically used the ILM pedagogy from his instructional toolbox and gave students grade incentives to correct their mistakes on the posttest. Students who took advantage of this opportunity and made posttest corrections not only showed gains on the revised posttest, they also performed better on a final exam question that focused on the same concepts. We note that even students who did not make corrections to their posttest had the opportunity to take advantage of learning from the solutions to the posttest provided for the class after students had the opportunity to correct their mistakes. However, their average score on the final exam question was lower than that of the group that took advantage of the ILM pedagogy and corrected their mistakes on the posttest. This finding is consistent with the previous study involving the ILM pedagogy spanning several years in which advanced undergraduate physics students in a similar QM course performed better on related tasks after being given incentives to correct their mistakes [63].

In summary, instructional pragmatism and being flexible about using various EBAE pedagogies as appropriate to suit the instructional situation at a given time dynamically can go a long way in improving teaching and learning in all physics courses.

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3.6 CHAPTER REFERENCES

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3.7 CHAPTER APPENDIX

(CQ1) *Choose all of the following statements about the product space for a system of* ***two spin-1/2 particles*** *in the* ***uncoupled representation*** *that are correct:*

I. *The dimensionality of the product space is the product of the dimensions of each particle's subspace, which is 2+2=4.*

II. $|s_1 m_{s1}\rangle \otimes |s_2, m_{s2}\rangle$ *is an appropriate form for the basis vectors.*

III. $\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$, $\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{-1}{2}\right\rangle$, *and* $\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{-1}{2}\right\rangle$ *are a complete set of basis vectors.*

a) *I only*

b) II only

c) *III only*

d) II and III only

e) None of the above

(CQ2) *Choose all of the following statements about the product space for a system of* ***two spin-1/2 particles*** *in the* ***uncoupled representation*** *that are correct:*

I. *Basis vector* $\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$ *is an eigenstate of* $\hat{S}_{1z}$ *such that:* $\hat{S}_{1z}\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle =$

$(\hat{S}_{1z} \otimes \mathbb{I})\left(\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle\right) = \left(\hat{S}_{1z}\left|\frac{1}{2},\frac{-1}{2}\right\rangle\right) \otimes \left(\mathbb{I}\left|\frac{1}{2},\frac{1}{2}\right\rangle\right) = \frac{-\hbar}{2}\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle.$

II. *Basis vector* $\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$ *is an eigenstate of* $\hat{S}_{2z}$ *such that:* $\hat{S}_{2z}\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle =$

$(\mathbb{I} \otimes \hat{S}_{2z})\left(\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle\right) = \left(\mathbb{I}\left|\frac{1}{2},\frac{-1}{2}\right\rangle\right) \otimes \left(\hat{S}_{2z}\left|\frac{1}{2},\frac{1}{2}\right\rangle\right) = \frac{\hbar}{2}\left(\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle\right).$

III. *Basis vector* $\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$ *is an eigenstate of* $\hat{S}_1^2$ *and* $\hat{S}_2^2$.

a) I only

b) II only

c) I and III only

d) II and III only

e) All of the above

(CQ3) *Consider the product space of a system of* ***two spin-1/2 particles*** *in the* *uncoupled*

<u>representation</u>. In this representation, it is most useful to write $\hat{S}_1 \cdot \hat{S}_2$ *as* $\frac{\hat{S}_{1-}\hat{S}_{2+}+\hat{S}_{1+}\hat{S}_{2-}}{2}+\hat{S}_{1z}\hat{S}_{2z}$. *Choose all of the following that are correct concerning scalar products. (Recall that these scalar products give the matrix elements of the* $\hat{S}_{1-}\hat{S}_{2+}$ *matrix in this basis).*

I. $\left\langle\frac{1}{2},\frac{-1}{2}\right| \otimes \left\langle\frac{1}{2},\frac{1}{2}\right| \hat{S}_{1-}\hat{S}_{2+} \left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{-1}{2}\right\rangle = (\left\langle\frac{1}{2},\frac{-1}{2}\right| \hat{S}_{1-} \left|\frac{1}{2},\frac{1}{2}\right\rangle)(\left\langle\frac{1}{2},\frac{1}{2}\right| \hat{S}_{2+} \left|\frac{1}{2},\frac{-1}{2}\right\rangle) = 0$

II. $\hat{S}_1 \cdot \hat{S}_2$ *will be diagonal in uncoupled representation*

III. $\left\langle\frac{1}{2},\frac{-1}{2}\right| \otimes \left\langle\frac{1}{2},\frac{1}{2}\right| \hat{S}_{1-}\hat{S}_{2+} \left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{-1}{2}\right\rangle = (\left\langle\frac{1}{2},\frac{-1}{2}\right| \hat{S}_{1-} \left|\frac{1}{2},\frac{1}{2}\right\rangle)(\left\langle\frac{1}{2},\frac{1}{2}\right| \hat{S}_{2+} \left|\frac{1}{2},\frac{-1}{2}\right\rangle) = \hbar^2$

IV. Some off-diagonal elements of $\hat{S}_1 \cdot \hat{S}_2$ *in the uncoupled representation are non-zero.*

- *a) II and III only*
- ***b) III and IV only***
- *c) II and III only*
- *d) I and IV only*
- *e) None of the above.*

(Class Discussion Notes)

Basis vectors in uncoupled representation are eigenstates of $\hat{S}_{1z}$, $\hat{S}_{2z}$, $\hat{S}_1^2$, *and* $\hat{S}_2^2$.

Basis vectors: $\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$, $\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{-1}{2}\right\rangle$, $\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle$, *and* $\left|\frac{1}{2},\frac{-1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{-1}{2}\right\rangle$

CQ4-CQ6 provided in the text are implemented here

(Class Discussion Notes)

Basis vectors in the coupled representation are eigenstates of $\hat{S}_z$, $\hat{S}_1^2$, $\hat{S}_2^2$, *and* $\hat{S}^2$.

Basis vectors: $|1,1\rangle$, $|1,0\rangle$, $|1,-1\rangle$, *and* $|0,0\rangle$

Compare and contrast uncoupled and coupled representations.

(CQ7) *Choose all of the following that are correct:*

I. *The product space for a system of* ***a spin-1 particle and a spin-3/2 particle*** *is 3+4=7 dimensional in both coupled and uncoupled representations.*

II. *The product space for a system of* ***a spin-1/2 particle and a spin-1 particle*** *is 2x3=6 dimensional in the coupled representation, but not in the uncoupled representation.*

III. *The product space for a system of* ***two spin-1 particles*** *is 3x3=9 dimensional in both coupled and uncoupled representations.*

a) I only

b) II only

c) III only

d) II and III only

e) None of the above

(CQ8) *Choose all of the following that are correct about the basis vectors in the* ***<u>uncoupled</u>*** *representation.*

I. *If* $s_1 = s_2 = 1,\ |1,-1\rangle \otimes |1,1\rangle,\ \ \left|1,\frac{1}{2}\right\rangle \otimes \left|1,\frac{1}{2}\right\rangle,$ *and* $|1,0\rangle \otimes |1,1\rangle$ *are appropriate basis vectors.*

II. *If* $s_1 = s_2 = \frac{3}{2},\ |0,0\rangle \otimes |1,1\rangle, |1,1\rangle \otimes |0,0\rangle,$ *and* $|1,0\rangle \otimes |1,0\rangle$ *are appropriate basis vectors.*

III. *If* $s_1 = 1,\ s_2 = \frac{3}{2},\ |1,0\rangle \otimes \left|\frac{3}{2},\frac{1}{2}\right\rangle, |1,0\rangle \otimes \left|\frac{3}{2},\frac{-3}{2}\right\rangle,$ *and* $|1,1\rangle \otimes \left|\frac{3}{2},\frac{3}{2}\right\rangle$ *are appropriate basis vectors.*

a) I only

b) II only

c) III only

d) II and III only

e) None of the above

(CQ9) *Choose all of the following that are correct about the basis vectors in the* ***<u>coupled</u>*** *representation:*

I. *For the product space of a system of* ***two spin-$\frac{3}{2}$ particles****, the possible values for the total spin* *quantum number s are 0, 1, 2, and 3, with some basis vectors being* $|3,-1\rangle$, $|0,-1\rangle$, *and* $|1,0\rangle$.

II. *For the product space of a system* ***of two spin-1 particles****, the possible values for s are 0, 1, and 2, with some examples of basis vectors being* $|1,-1\rangle$, $|2,1\rangle$, *and* $|0,0\rangle$.

III. *For the product space of a system of* ***a spin-1 particle and a spin-3/2 particle****, the possible values for s are 0, 1/2, 3/2, and 5/2 , with some basis vectors being* $\left|\frac{5}{2},\frac{-3}{2}\right\rangle$, $\left|\frac{1}{2},\frac{-1}{2}\right\rangle$, *and* $\left|\frac{3}{2},\frac{1}{2}\right\rangle$.

a) I only

b) II only

c) III only

d) II and III only

e) None of the above

(CQ10) *Choose all of the following that are correct about the product space of a system of* ***a spin-*** $\boldsymbol{\frac{1}{2}}$ ***particle and a spin-1 particle*** *with the basis vectors in the* ***coupled*** *representation:*

I. *The possible values for the total spin quantum number s are* $\frac{1}{2}$ *and* $\frac{3}{2}$, *with* $m_s = \frac{1}{2}, \frac{-1}{2}, \frac{3}{2}, \frac{-3}{2}$ *for* $s = \frac{3}{2}$ *and* $m_s = \frac{1}{2}, \frac{-1}{2}$ *for* $s = \frac{1}{2}$.

II. *This is a 4-dimensional product space with basis vectors* $\left|\frac{1}{2},\frac{1}{2}\right\rangle$, $\left|\frac{1}{2},-\frac{1}{2}\right\rangle$, $\left|\frac{3}{2},\frac{3}{2}\right\rangle$, *and* $\left|\frac{3}{2},-\frac{3}{2}\right\rangle$ *because the possible values of* $m_s = \frac{1}{2}, \frac{-1}{2}, \frac{3}{2}, \frac{-3}{2}$.

III. *This is a 6-dimensional product space with basis vectors* $\left|\frac{1}{2},\frac{1}{2}\right\rangle$, $\left|\frac{1}{2},-\frac{1}{2}\right\rangle$, $\left|\frac{3}{2},\frac{3}{2}\right\rangle$, $\left|\frac{3}{2},-\frac{3}{2}\right\rangle$, $\left|\frac{3}{2},\frac{1}{2}\right\rangle$, *and* $\left|\frac{3}{2},-\frac{1}{2}\right\rangle$ *because the values of* $m_s = \frac{1}{2}, \frac{-1}{2}, \frac{3}{2}, \frac{-3}{2}$ *for* $s = \frac{3}{2}$ *and* $m_s = \frac{1}{2}, \frac{-1}{2}$ *for* $s = \frac{1}{2}$.

a) I only

b) II only

c) I and II only

d) I and III only

e) All of the above.

(Class Discussion Notes)

What are the values of the total spin quantum number and the z component of the total spin quantum number, $\boldsymbol{s}$ *and* m_s *, respectively, for the product space of a system of* ***a spin-$\frac{1}{2}$ particle and a spin-1 particle****, e.g., for writing the basis states in the* ***<u>coupled</u>*** *representation?*

What is the dimensionality of this product space?

(CQ11) *When working with a given operator(s), it is useful to consider which representation is more <u>convenient</u> to work in. Choose all of the following statements that are correct about choosing a convenient basis to work in:*

I. *Basis vectors in uncoupled representation are eigenstates of* $\hat{S}_{1z}$*, and* $\hat{S}_{2z}$*, making a convenient basis for operators that commute with* $\hat{S}_{1z}$*, and* $\hat{S}_{2z}$*.*

II. *Basis vectors in the coupled representation are eigenstates of* $\hat{S}_z$ *and* $\hat{S}^2$*, making a* *convenient basis for operators that commute with $\hat{S}_z$ and $\hat{S}^2$.*

III. *Basis vectors in both couple and uncoupled representations are eigenstates of $\hat{S}_1^2$ and $\hat{S}_2^2$, making either convenient bases for operators that commute with $\hat{S}_1^2$ and $\hat{S}_2^2$.*

a) *I only*

b) *II only*

c) *I and II only*

d) *I and III only*

e) All of the above

(CQ12) *Consider the Hamiltonian $\hat{H} = C\hat{S}_1 \cdot \hat{S}_2$. Choose all of the following statements that are correct about this operator acting on the basis vectors for the product space of a system of* ***two identical particles with non-zero spin:***

I. *The Hamiltonian matrix is diagonal in the coupled basis because the basis vectors in coupled representation are eigenstates of the operators $\hat{S}^2$, $\hat{S}_1^2$, and $\hat{S}_2^2$*

II. *The Hamiltonian matrix is diagonal in the uncoupled basis because the basis vectors in uncoupled representation are eigenstates of the operators $\hat{S}_{1+}, \hat{S}_{1-}, \hat{S}_{2+}, \hat{S}_{2-}, \hat{S}_{1z}$, and $\hat{S}_{2z}$*

III. *For a system of* ***two identical spin-1/2 particles****, this Hamiltonian matrix is 4-by-4 in either the coupled representation or uncoupled representation.*

a) *I only*

b) II only

c) I and II only

d) I and III only

e) All of the above.

(Class Discussion Notes)

For the Hamiltonian $\widehat{H} = C\hat{S}_1 \cdot \hat{S}_2$, which representation is <u>convenient</u>? Uncoupled, coupled, both, or neither? Why?

*For the Hamiltonian $\widehat{H} = C\hat{S}_1 \cdot \hat{S}_2$, the Hamiltonian is diagonal in the **coupled representation**, but not the uncoupled representation. The **coupled representation is** <u>convenient</u>.*

(CQ13) *Consider the Hamiltonian $\widehat{H} = C(\hat{S}_{1z} + \hat{S}_{2z})$. Choose all of the following statements that are correct about this operator acting on basis vectors for the product space of a system of **two identical particles with non-zero spin:***

I. *The Hamiltonian matrix is diagonal in the coupled basis because the basis vectors in the coupled representation are eigenstates of the operator $\hat{S}_z = (\hat{S}_{1z} + \hat{S}_{2z})$*

II. *The Hamiltonian matrix is diagonal in the uncoupled basis because the basis vectors in the uncoupled representation are eigenstates of the operators $\hat{S}_{1z}$ and $\hat{S}_{2z}$*

III. *For a system of **two identical spin-1/2 particles**, this Hamiltonian matrix is 4-by-4 whether* *the coupled representation or uncoupled representation is chosen.*

a) *I only*
b) *II only*
c) *I and II only*
d) *I and III only*
e) ***All of the above***.

(Class Discussion Notes)

For the Hamiltonian $\hat{H} = C(\hat{S}_{1z} + \hat{S}_{2z})$, *which representation is* *convenient*? *Uncoupled, coupled, both, or neither? Why?*

For the Hamiltonian $\hat{H} = C(\hat{S}_{1z} + \hat{S}_{2z})$, *the Hamiltonian is diagonal in both the* ***coupled and uncoupled representations***.

Both the ***coupled and uncoupled representation*** *are* *convenient*.

4.0 DEVELOPMENT, VALIDATION, AND IN-CLASS EVALUATION OF A SEQUENCE OF CLICKER QUESTIONS ON LARMOR PRECESSION OF SPIN IN QUANTUM MECHANICS

4.1 INTRODUCTION AND BACKGROUND

Clicker questions (also known as concept tests) are conceptual multiple-choice questions typically administered in the classroom to engage students in the learning process and obtain feedback about their learning via a live feedback system called clickers [1-13]. Integration of peer interaction with lectures via clicker questions has been popularized in the physics community by Mazur [2]. In Mazur's approach, the instructor poses conceptual, multiple-choice clicker questions to students which are integrated throughout the lecture. Students first answer each clicker question individually, which requires them to take a stance regarding their thoughts about the concept(s) involved. Students then discuss their answers to the questions with their peers and learn by articulating their thought processes and assimilating their thoughts with those of the peers. Then after the peer discussion, they answer the question again using clickers followed by a general class discussion about those concepts in which both students and the instructor participate. The feedback that the instructor obtains is also valuable because the instructor has an estimate of the prevalence of student common difficulties and the fraction of the class that has understood the concepts and can apply them in the context in which the clicker questions are posed. The use of clickers keeps students alert during lectures and helps them monitor their learning. Clicker questions can be used in the classroom in different situations, e.g., they can be interspersed within lectures to evaluate student learning in each segment of a class focusing on a concept, at the end of a class or to review materials from previous classes at the beginning of a class.

While clicker questions for introductory [2] and upper-level physics such as quantum mechanics [14] have been developed, there have been very few documented efforts [15] toward a systematic development and validation of clicker question sequences (CQSs), e.g., question sequences on a given concept that can be used in a few class periods when students learn the concepts and that build on each other effectively and strive to help students organize, extend and repair their knowledge structure pertaining to the topic.

Here we discuss the development, validation and in-class implementation of a CQS to help students develop conceptual understanding of the Larmor precession of spin in quantum mechanics (QM) that was developed for students in upper-level undergraduate QM courses taken by physics juniors and seniors. The CQS was developed by taking advantage of the learning goals and inquiry-based guided learning sequences in a research-validated Quantum Interactive Learning Tutorial (QuILT) on this topic [16] as well as by refining, fine-tuning and adding to the existing clicker questions from our group which have been individually validated previously [14]. The CQS can be used in class either separately from the QuILT or synergistically with the corresponding QuILT [16] if students engage with the QuILT after the CQS as another opportunity to reinforce the concepts learned.

4.2 LEARNING GOALS AND METHODOLOGY

The learning goals and inquiry-based learning sequences in the QuILT, which guided the development and sequencing of the CQS questions, were developed using extensive research on student difficulties with these concepts as a guide and cognitive task analysis from an expert perspective.

4.2.1 Learning Goals

One The first learning goal of the CQS (consistent with the QuILT) is that students should be able to unpack the consequence of Ehrenfest's theorem that the time dependence of the expectation value of any observable whose corresponding Hermitian operator commutes with the Hamiltonian is zero regardless of the state of the quantum system. This is highlighted throughout the CQS by students considering the expectation value of $\hat{S}_Z$ and realizing that it is always time independent regardless of the quantum state for the Hamiltonian $\widehat{H} = -\gamma B_0 \hat{S}_z$ since $\hat{S}_Z$ commutes with the Hamiltonian. The second learning goal is for students to learn another application of Ehrenfest's theorem in that the expectation value of any observable (which does not have explicit time-dependence) is not dependent on time when the initial state is a stationary state. In particular, if the system is in a stationary state (i.e., an eigenstate of the Hamiltonian) the expectation values of all observables are time independent, rather than just those observables whose corresponding operators commute with the Hamiltonian. Throughout the CQS, stationary states are eigenstates of $\hat{S}_Z$, challenging students to recognize that these are eigenstates of the Hamiltonian so the expectation values of $\hat{S}_X$ and $\hat{S}_Y$ are also time-independent. Finally, the third learning goal of the CQS is for students to be able to distinguish between stationary states and eigenstates of Hermitian operators that do not commute with the Hamiltonian (e.g., those corresponding to observables other than energy). For the Hamiltonian $\widehat{H} = -\gamma B_0 \hat{S}_z$, students should learn that an eigenstate of either $\hat{S}_X$ and $\hat{S}_Y$ is not a stationary state, unlike a system in an eigenstate of $\hat{S}_Z$.

4.2.2 Development and Validation

Based upon the learning goals delineated in the QuILT, questions in the Larmor precession of spin CQS were developed or adapted from prior validated clicker questions and sequenced to balance difficulties, avoid change of both concept and context between consecutive questions as appropriate in order to avoid a cognitive overload, and include a mix of abstract and concrete questions to help students develop a good grasp of relevant concepts. The validation was an iterative process.

After the initial development of the Larmor precession of spin CQS using the learning goals and inquiry-based guided learning sequences in the QuILT and some existing individually validated clicker questions, we iterated the CQS with three physics faculty members who provided valuable feedback on fine-tuning and refining both the CQS as a whole and some new questions that were developed and adapted with existing ones to ensure that the questions were unambiguously worded and build on each other based upon the learning goals. We also conducted individual think-aloud interviews with four advanced students who had learned these concepts via traditional lecture-based instruction in relevant concepts to ensure that they interpreted the CQS questions as intended and the sequencing of the questions provided appropriate scaffolding support to students.

The final version of the Larmor precession of spin CQS has 6 questions, which can be integrated with lectures in which these relevant concepts are covered in a variety of ways based upon the instructor’s preferences. In particular, they can be interspersed with lecture or posed together depending, e.g., upon whether they are integrated with lectures similar to Mazur’s approach, used at the end of each class or used to review concepts after students have learned via lectures everything related to Larmor precession of spin that the instructor wanted to teach.

The first two questions in the CQS, CQ1andCQ2, begin by addressing the time-development of a state that is initially an energy eigenstate or not initially an energy eigenstate. This calls on students' prior knowledge about the time development of a state before addressing general characteristics of the time dependence of an expectation value of $\hat{\vec{S}}$ in CQ3 and CQ4. CQ5 addresses the time dependence of expectation value for different components of the spin for a state that is not an eigenstate of the Hamiltonian, but rather an eigenstate of the *x*-component of the spin angular momentum, $\hat{S}_X$. The sequence then concludes by contrasting CQ5 with a similar question CQ6 which is for a system initially in an energy eigenstate.

The questions in the CQS are as follows:

(CQ1) *An electron in a magnetic field $\vec{B} = B_0\hat{z}$ is initially in a spin state $|\chi(0)\rangle = |\uparrow\rangle_z$. Which of the following equations correctly represents the state $|\chi(t)\rangle$ of the electron after time t? The Hamiltonian operator is $\hat{H} = -\gamma B_0 \hat{S}_z$.*

a) $|\chi(t)\rangle = |\uparrow\rangle_z$

b) $\boldsymbol{|\chi(t)\rangle = e^{i\gamma B_0 t/2}|\uparrow\rangle_z}$

c) $|\chi(t)\rangle = e^{i\gamma B_0 t/2}|\uparrow\rangle_z + e^{-i\gamma B_0 t/2}|\downarrow\rangle_z$

d) $|\chi(t)\rangle = ae^{i\gamma B_0 t/2}|\uparrow\rangle_z + be^{i\gamma B_0 t/2}|\downarrow\rangle_z$

e) None of the above.

(CQ2) *An electron in a magnetic field* $\vec{B} = B_0\hat{z}$ *is initially in a spin state* $|\chi(0)\rangle = a|\uparrow\rangle_z + b|\downarrow\rangle_z$*. Which of the following equations correctly represents the state* $|\chi(t)\rangle$ *of the electron after time t? The Hamiltonian operator is* $\hat{H} = -\gamma B_0 \hat{S}_z$.

a) $|\chi(t)\rangle = e^{i\gamma B_0 t/2}(a|\uparrow\rangle_z + b|\downarrow\rangle_z)$

b) $|\chi(t)\rangle = e^{-i\gamma B_0 t/2}(a|\uparrow\rangle_z + b|\downarrow\rangle_z)$

c) $|\chi(t)\rangle = e^{i\gamma B_0 t/2}((a+b)|\uparrow\rangle_z + (a-b)|\downarrow\rangle_z)$

d) $|\boldsymbol{\chi(t)}\rangle = \boldsymbol{a e^{i\gamma B_0 t/2}}|\uparrow\rangle_{\boldsymbol{z}} + \boldsymbol{b e^{-i\gamma B_0 t/2}}|\downarrow\rangle_{\boldsymbol{z}}$

e) None of the above

(CQ3) *Choose all of the following statements that are true about the expectation value* $\langle \hat{\vec{S}} \rangle$ *for an electron in a magnetic field* $\vec{B} = B_0\hat{z}$ *in the state* $|\chi(t)\rangle$ *when the initial state is* ***NOT*** $|\uparrow\rangle_z$ *or* $|\downarrow\rangle_z$*. The Hamiltonian operator is* $\hat{H} = -\gamma B_0 \hat{S}_z$.

I. The z-component of $\langle \hat{\vec{S}} \rangle$*, i.e.* $\langle \hat{S}_Z \rangle$*, is time-independent.*

II. The x- and y-components of $\langle \hat{\vec{S}} \rangle$ *change with time. When the magnitude of* $\langle \hat{S}_X \rangle$ *is a maximum, the magnitude of* $\langle \hat{S}_Y \rangle$ *is a minimum, and vice versa.*

III. The magnitudes of the maximum values of $\langle \hat{S}_X \rangle$ *and* $\langle \hat{S}_Y \rangle$ *are the same.*

a) I only

b) I and II only

c) I and IIV only

d) II and III only

e) All of the above.

(CQ4) *Choose all of the following statements that are true about the expectation value $\langle\hat{\vec{S}}\rangle$ for an electron in a magnetic field $\vec{B} = B_0\hat{z}$ in the state $|\chi(t)\rangle$ when the initial state is* ***NOT*** *$|\uparrow\rangle_z$ or $|\downarrow\rangle_z$. The Hamiltonian operator is $\hat{H} = -\gamma B_0\hat{S}_z$.*

I. The vector $\langle\hat{\vec{S}}\rangle$ can be thought to be precessing about the z-axis at a non-zero angle.

II. The vector $\langle\hat{\vec{S}}\rangle$ can be though to be precessing about the z-axis at a frequency $\omega = \gamma B_0$.

I. All three components of vector $\langle\hat{\vec{S}}\rangle$ change as it precesses about the z-axis.

a) I only

b) I and II only

c) I and III only

d) II and III only

e) All of the above.

(CQ5) *Suppose an electron in a magnetic field $\vec{B} = B_0\hat{z}$ is initially in an eigenstate of the x-component of spin angular momentum operator, i.e. $\hat{S}_X$. The Hamiltonian operator is $\hat{H} = -\gamma B_0\hat{S}_z$. Choose all of the following statements that are correct.*

I. The expectation value $\langle\hat{S}_X\rangle$ depends on time.

II. The expectation value $\langle \hat{S}_Y \rangle$ depends on time.

III. The expectation value $\langle \hat{S}_Z \rangle$ depends on time.

a) I only

b) I and II only

c) I and III only

d) II and III only

e) All of the above.

(CQ6) *Suppose an electron in a magnetic field $\vec{B} = B_0\hat{z}$ is initially in an eigenstate of the z-component of spin angular momentum operator, i.e. $\hat{S}_Z$. The Hamiltonian operator is $\hat{H} = -\gamma B_0 \hat{S}_z$. Choose all of the following statements that are correct.*

IV. The expectation value $\langle \hat{S}_X \rangle$ depends on time.

V. The expectation value $\langle \hat{S}_Y \rangle$ depends on time.

VI. The expectation value $\langle \hat{S}_Z \rangle$ depends on time.

a) I only

b) I and II only

c) I and III only

d) II and III only

e) None of the above.

4.2.3 In-class implementation

A The final version of the CQS on the Larmor precession of spin was implemented with peer discussion [2-4] in two upper-level undergraduate QM classes at a large research university (Pitt) after traditional lecture-based instruction in relevant concepts in two consecutive years. Prior to the implementation of the CQS in both classes with peer interaction, students took a pretest after traditional lecture-based instruction. The pre/postests were developed and validated by Brown and Singh [16] to measure comprehension of the concepts related to the time-dependence of expectation values of observables in the context of the Larmor precession of spin. The CQS was implemented right after the pretest in one class period with peer interaction. The posttest was administered during the following week to measure the impact of the CQS.

On the pretest and posttest, students were given that the Hamiltonian of the system is $\widehat{H} = -\gamma B_0 \hat{S}_z$ with questions 1-3 being analogous but different and questions 4-6 being identical. In particular, an electron is initially in an eigenstate of $\hat{S}_x$ ($\hat{S}_Y$ on the posttest) in questions 1-3, and students are asked if the expectation value of $\hat{S}_x$, $\hat{S}_Y$, and $\hat{S}_Z$ respectively depend on time. Students are also expected to explain their reasoning. These questions primarily focus on the first and third learning goals. Question 4 presents the following conversation between two students about an electron initially in an eigenstate of $\hat{S}_x$ ($\hat{S}_Y$ on the posttest) and asks with whom they agree. This question addresses the first and third learning goals.

Andy: *The electron will NOT be in an eigenstate of* $\hat{S}_x$ *forever because the state will evolve in time.*

Caroline: *I disagree. If a system is in an eigenstate of an operator corresponding to a physical observable, it stays in that state forever unless a perturbation is applied.*

Questions 5 asks students if the expectation value of $\hat{S}_Y$ is time dependent if the initial state of the system is an eigenstate of $\hat{S}_Z$ (i.e., an eigenstate of the Hamiltonian or stationary state). Then, question 6 asks if there is precession around the z-axis for an electron initially in an eigenstate of $\hat{S}_Y$, and if so, to give an example of a situation in which there would be no precession. Both of these questions deal with the second and third learning goals. All questions ask students to justify their answers. Partial credit was awarded to students who answered correctly, but with no or inadequate justification, consistent with the agreed upon rubric. Interrater reliability between the two researchers who graded all pre/posttests was above 95%.

4.3 IN-CLASS IMPLEMENTATION RESULTS

Tables 4.1-4.3 compare average pre/posttest performances of students on each question in the upper-level QM course from the same large research university in two different years after traditional lecture-based instruction (pretest) and on the posttest after students had engaged with the CQS with peer instruction on the Larmor precession of spin (Table 4.1-4.2 are for the two classes separately and Table 4.3 is for the two classes combined). The normalized gain (or gain) is calculated as $g = (post\% - pre\%)/(100\% - pre\%)$ [17]. Similarly, the effect size is calculated for all questions in all tables. Effect size is calculated as Cohen's $d = (\mu_{post} - \mu_{pre})/\sigma_{pooled}$ where μ_i is the mean of group i and the pooled standard deviation is $\sigma_{pooled} = \sqrt{(\sigma_{pre}{}^2 + \sigma_{post}{}^2)/2}$ [18].

Table 4.1 Comparison of mean pre/posttest scores on each question, normalized gains and effect sizes for upper-level undergraduate QM students in class A who engaged with the CQS on Larmor precession of spin concepts (N=17).

Question	Pretest Mean	Posttest Mean	Normalized Gain (g)	Effect Size (d)
1	22%	75%	0.68	0.69
2	47%	84%	0.71	0.54
3	19%	72%	0.65	0.66
4	31%	81%	0.73	0.62
5	13%	47%	0.39	0.42
6	34%	75%	0.62	0.50

Table 4.2 Comparison of mean pre/posttest scores on each question, normalized gains and effect sizes for upper-level undergraduate QM students in class B who engaged with the CQS on Larmor precession of spin concepts (N=39).

Question	Pretest Mean	Posttest Mean	Normalized Gain (g)	Effect Size (d)
1	50%	92%	0.85	0.56
2	67%	94%	0.82	0.48
3	52%	95%	0.91	0.61
4	41%	79%	0.64	0.43
5	38%	82%	0.71	0.51
6	56%	85%	0.66	0.35

Table 4.3 Comparison of mean pre/posttest scores on each question, normalized gains and effect sizes for upper-level undergraduate QM students in both class A and class B combined who engaged with the CQS on Larmor precession of spin concepts (N=56).

Question	Pretest Mean	Posttest Mean	Normalized Gain (g)	Effect Size (d)
1	41%	87%	0.78	0.59
2	60%	91%	0.77	0.49
3	41%	88%	0.79	0.59
4	38%	80%	0.67	0.49
5	30%	70%	0.58	0.46
6	49%	82%	0.64	0.40

All three tables show moderate effect sizes from pre to posttest on each of the questions, with all effect sizes above 0.3, and some even nearing 0.7. Additionally, all normalized gains exceed 0.3, with most falling in the range of 0.6-0.9. Despite varied pretest scores for the two classes on different questions, posttest scores for both classes on most questions demonstrate that the CQS is effective in addressing the learning goals.

Although the two groups of upper-level physics majors in the QM course from the same university in two consecutive years are different, the difference in pretest scores between two classes may also be a reflection of the difference between the effectiveness of traditional instruction of the two instructors. On a positive note, the posttest scores for both groups are robust. We note that overall the CQS implementation was consistent between the two years, and both instructors provided the same class participation credit for clicker questions and low-stakes testing credit for students to take the pre-/posttests. However, no constraints were placed on instructors' teaching of the topic in class prior to the implementation of the CQS, as the CQS in this implementation is meant to act primarily as a "second coat" to reinforce learning. Moreover, possible differences between the instructors may include, but are certainly not limited to, the differences in pedagogy and the time spent in lecture on the topic.

Since the researchers did not have control over traditional instruction, we focus on the posttest scores after the CQS. Tables 4.1 and 4.2 show that the difference in pretest scores between the two classes is also followed by a corresponding difference in posttest scores after the CQS. These differences in posttest scores may indicate that the prior knowledge of the material (or the first coat) does affect how well students learn from the CQS implementation with peer instruction. In particular, Class B, which exhibited higher pretest scores than Class A on all test questions, also exhibited higher posttest scores on five of the six test questions, and exhibited comparable posttest scores on question 4. From this comparison, we conclude that the CQS did not eliminate the performance gap in pretest resulting from differences in knowledge after traditional instruction in the two classes and before students engaged with the CQS. It is possible that certain threshold knowledge may be prerequisite for optimal learning from the CQS particularly because peer instruction was involved and students can meaningfully communicate and learn from each other only if together they have certain threshold knowledge.

However, we note that those higher pretest scores of Class B in Table 4.2 do not exceed the posttest scores of Class A in Table 4.1. While the highest average score for Class B on the pretest is still below 70%, five of the six posttest scores for Class A exceed 70%. From this comparison, we conclude that, regardless of the effectiveness of traditional lecture-based instruction for a given instructor, students still had something to gain pertaining to the time-dependence of expectation values from the CQS.

Moreover, as shown in Table 4.3, overall (averaging over the two classes), the CQS was effective in addressing its learning goals. On average, student performance on test questions range from 30-60% on the pretest, showing that there is much room for improvement after traditional instruction. After the implementation of the CQS, average scores on test questions exceeded 70% on the posttest and exceed 90% on questions 1-3.

Difficulty with question 5 was the most common among students, with Class A averaging below 50% on the question even after the CQS implementation. This suggests that there is still room for improving the CQS when dealing with the second learning goal in order for students to understand the special role of the stationary states in different contexts. This was a learning goal addressed by both questions 5 and 6 on the pretest and posttest, but the difference in performance suggests that students with less prior knowledge (Class A) failed to perform on question 5, even though they averaged above 75% on question 6, which provides more scaffolding. In order to address this difficulty, the CQS may be improved by adding another question later in the CQS that more directly addresses this second learning goal. This question could provide an opportunity to wean students from the scaffolding provided in prior questions related to this learning goal and may allow for more effective learning on future implementations of this CQS.

4.4 SUMMARY

Clicker questions are relatively easy to implement in the classroom alongside more traditional lecture-based instruction. We developed and validated a clicker question sequence related to the time-dependence of expectation values in the context of Larmor precession of spin that continually builds on students' knowledge as they engage with different questions in the CQS after traditional instruction in relevant concepts. Throughout the development and validation which was an iterative process, many students and instructors provided feedback several times. The in-class implementation of the CQS in two upper-level quantum mechanics classes shows moderate effect sizes for gains in students' performance from the pretest to posttest suggesting this CQS is effective in helping students learn these concepts. The differences in the pretest scores in the two classes could be due to the differences in the students and the instructors and the effectiveness of their traditional instruction over which the researchers did not have any control. However, the posttest scores on all questions in both classes were reasonable, suggesting that the CQS is effective regardless of efficacy of an instructor's traditional lecture-based instruction. Moreover, comparison of the pre/posttest scores on each question for the two classes in which students engaged with the CQS may shed some light on the role of prior knowledge upon which students can build as they engage with the questions in the CQS. In particular, the average posttest scores were generally higher on each question for the class which had a higher pretest scores. This issue will be investigated further in future implementation.

4.5 ACKNOWLEDGEMENTS

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5.0 STUDENT UNDERSTANDING OF FERMI ENERGY, THE FERMI-DIRAC DISTRIBUTION, AND TOTAL ELECTRONIC ENERGY OF A FREE ELECTRON GAS

5.1 INTRODUCTION

In the past two decades, many investigations have focused on improving student learning of quantum mechanics (QM) e.g., see Ref. [1-9]. We have been deeply involved in such investigations and are using the research on student difficulties as a guide to develop research-validated learning tools [10-33].

5.1.1 Goals of this investigation

While the Fermi energy, the Fermi-Dirac distribution and total electronic energy of a free electron gas are important concepts [34] taught in advanced quantum and statistical mechanics courses, there has been little work done on investigating student difficulties with these concepts. Here we discuss an investigation of the difficulties that upper-level physics undergraduates in a QM course and physics graduate students after quantum and statistical mechanics core courses have with these concepts after they had learned them in their respective courses. These difficulties were probed by administering written conceptual and quantitative questions to undergraduate students and asking some students in undergraduate and graduate courses to answer the questions while thinking aloud [35] in one-on-one interviews. We find that advanced students have many common difficulties with these concepts after traditional instruction. We also discuss the impact of a clicker question sequence (CQS) on undergraduate student performance on these topics. The CQS was developed and validated to help students develop a better grasp of these concepts. The implementation of the CQS in **an** upper-level undergraduate QM **course** shows that while engaging with the CQS reduced these difficulties, many advance students continued to struggle with these challenging concepts.

5.1.2 Background on relevant topics

The free electron gas [34] is a commonly taught model of solids (metals) in a two-semester upper-level undergraduate and core graduate quantum mechanics course. This model ignores many realities of real metals like the electron charge and the underlying lattice. The main consideration is the Pauli exclusion principle, which requires electrons to occupy distinct single-particle states. In this non-interacting fermionic model in three spatial dimensions, electrons can be considered to move freely in a three dimensional infinite rectangular box. Since the size of a solid is macroscopic and the number of electrons is very large (of the order of Avogadro's number), the actual shape of the solid is not important for determining the properties of the solid, and the free electron gas model explains many qualitative properties of conductors reasonably well [34].

Although the concepts of Fermi energy and density of states are defined more broadly, these are two key concepts advanced students often learn for the first time in the context of the free electron gas model of a solid. The Fermi energy E_f is the energy of the highest occupied state at absolute zero temperature $T = 0\ K$. The density of states of the system $D(\epsilon)$ is the number of states per interval of energy for a given energy ϵ. The concepts of Fermi energy and density of states can be used to calculate the total electronic energy of a solid at $T = 0\ K$, i.e., $E_{tot} = \int_0^{E_F} D(\epsilon)\epsilon\, d\epsilon$.

In quantum statistical mechanics [34], the concept of the distribution function, $n(\epsilon)$, which is defined as the average number of particles in a given single-particle state with energy ϵ at a given temperature T, becomes important. At $T = 0\ K$, the Fermi-Dirac (FD) distribution function for a non-interacting fermionic system, e.g., electrons discussed here, is a step function such that all single-particle states below the Fermi energy are completely filled and all states above the Fermi energy are empty. However, as the temperature increases, the probability of occupying higher single particle energy states increases and at very high temperature when the de Broglie wavelength is so small that the wavefunctions of different electrons do not overlap, the Fermi-Dirac distribution function reduces to the Maxwell-Boltzmann (MB) distribution function, which is an exponential function of energy ϵ. The Fermi-Dirac distribution function is $n_{FD}(\epsilon) = \frac{1}{e^{\frac{\epsilon-\mu(T)}{k_B T}}+1}$, where μ is the chemical potential, defined as the energy required to add an extra particle to the system. The chemical potential μ depends on temperature T and is equal to the Fermi energy at $T = 0\ K$. The total electronic energy of the system at temperature T is given by $E_{tot} = \int_0^{\infty} n(\epsilon)\, D(\epsilon)\epsilon\, d\epsilon$. For comparison, the Bose-Einstein (BE) distribution function for a bosonic system is given by $n_{BE}(\epsilon) = \frac{1}{e^{\frac{\epsilon-\mu(T)}{k_B T}}-1}$. There are no constraints on the number of bosons in a given single-particle state.

5.1.3 Background on Clicker Questions

Clicker questions are conceptual multiple-choice questions that are typically administered in the classroom to engage students in the learning process and obtain feedback about their learning via a live feedback system called clickers [36-37]. Integration of peer interaction with lectures via clicker questions has been popularized in the physics community by Mazur [36]. In Mazur's approach, the instructor poses conceptual, multiple-choice clicker questions to students which are integrated throughout the lecture. Students first answer each clicker question individually, which requires them to take a stance regarding their thoughts about the concepts involved. Students then discuss their answers to the questions with their peers and learn by articulating their thought processes and assimilating their thoughts with those of the peers. After the peer discussion, they answer the question again using clickers followed by a general class discussion about those concepts in which both students and the instructor participate. The feedback that the instructor obtains is also valuable because the instructor has an estimate of the prevalence of student common difficulties and the fraction of the class that has understood the concepts at least in the context in which the clicker questions were posed. The use of clickers keeps students alert during lectures and helps them monitor their learning. Clicker questions can be used in the classroom in different situations, e.g., they can be interspersed within lecture to evaluate student learning in each segment of a class focusing on a concept, at the end of a class, or to review materials from previous classes at the beginning of a class. They can also be used in a Just-in-Time-Teaching class [38-39] at any time to engage students in learning based upon what they may have been asked to learn outside of the class.

5.1.4 Clicker Question Sequence on Fermi energy, total electronic energy, and Fermi-Dirac distribution function

While clicker questions for introductory [36-37] and upper-level QM [39-40] have been developed, there have been very few efforts [41] toward a systematic development and implementation of clicker question sequences (CQSs), e.g., those on a given concept in which the questions build on each other effectively to help students organize their knowledge. Here we discuss how student performance on questions probing their understanding of the Fermi energy and total electronic energy of a free electron gas, and of the Fermi-Dirac distribution function, in an upper-level undergraduate QM course was impacted by a CQS focusing on these concepts. This CQS was developed and validated by contemplating the learning objectives, and by refining and fine-tuning existing clicker questions or developing new questions. The learning objectives related to Fermi energy include helping students learn to calculate the Fermi energy in terms of the free electron number density and realize that the Fermi energy is not an extensive quantity. The learning objectives related to the total electronic energy of a free electron gas include helping students learn to calculate the total electronic energy and realize that this quantity is extensive and therefore scales with the size of the system. The learning objectives related to the distribution functions include preparing students to be able to write an expression for them, be able to distinguish the Fermi-Dirac distribution function from the Bose-Einstein and Maxwell-Boltzmann distribution functions, be able to explain when the Fermi-Dirac (and Bose-Einstein) distribution functions will approach the Maxwell-Boltzmann distribution function, and be able to graphically represent the Fermi-Dirac distribution function at $T = 0\,K$ and at $T > 0\,K$. The validation was an iterative process. The three authors met to holistically examine the instructional materials from the past few years on these topics in an upper-level undergraduate QM course at a large university, which included existing clicker questions on these concepts. In particular, the questions in the CQS were developed or adapted from prior clicker questions and sequenced to balance difficulties, avoid change of both concept and context between consecutive questions as appropriate in order to avoid a cognitive overload, and include a mix of abstract and concrete questions to help students develop a good grasp of the concepts. After the initial development of the CQS, we iterated the CQS with three physics faculty members who provided valuable feedback on fine-tuning and refining both the CQS as a whole and individual questions that were developed and adapted from existing clicker questions to ensure that the questions were unambiguously worded and build on each other based upon the learning objectives. We also conducted think-aloud interviews [35] with advanced students who had learned these concepts via traditional lecture-based instruction to ensure that they interpreted the CQS questions as intended and the sequencing of questions provided appropriate guidance to help them learn relevant concepts.

5.2 METHODOLOGY

The students who participated in this study were upper-level physics undergraduates in a second semester junior/senior-level QM course and graduate students who had taken graduate core quantum and statistical mechanics courses. Both the undergraduate and graduate courses typically have 10-20 students each year. The undergraduate students had also taken the first semester of QM in the preceding semester and a majority of them had also taken or were concurrently taking a one-semester undergraduate thermodynamics and statistical mechanics course. The student difficulties were investigated by administering open-ended questions in written form to undergraduate students in the QM course after traditional lecture-based instruction in relevant concepts (we will call this pretest) and also after students had engaged with the CQS on relevant concepts (we will call this posttest). As noted earlier, the CQS questions were validated with the help of physics instructors who had taught QM and/or statistical mechanics courses several times (the questions were iterated with them to ensure that they were robust and interpreted unambiguously by physics experts) and students to ensure, e.g., that they interpreted the questions as intended.

In addition to written tests, we also conducted individual semi-structured interviews with a subset of students in the undergraduate course and with graduate students after they had completed core graduate QM and statistical mechanics courses in which relevant concepts were covered. Individual interviews were conducted using a think-aloud protocol [35] to better understand the rationale for student responses. During the interviews, similar to the in-class written administration in the undergraduate course, students were first given the open-ended question after traditional instruction (pretest), then they worked through the CQS, and then they were given the open-ended questions again as a posttest. The testing materials were developed and validated to assess student understanding of these concepts based upon the learning objectives delineated earlier. During these semi-structured interviews, students were asked to verbalize their thought processes while they answered the questions. They read the questions and answered them to the best of their ability without being disturbed. We prompted them to think aloud [35] if they were quiet for a long time. After students had finished answering a particular question to the best of their ability, we asked them to further clarify and elaborate issues that they had not clearly addressed earlier.

The final version of the CQS questions pertaining to this series on the free electron gas at T = 0 K has 11 questions (first 11 questions as shown in the Appendix) but the only relevant questions for the pre/posttests are CQ1-CQ7 and CQ10 (note that CQ11 pertaining to the two dimensional free-electron gas was not administered to students in this study but it is included here as an instructional resource). The last six CQS questions in the Appendix pertain to T > 0 K. Since the instructor used the textbook by Griffiths [34], the notation and discussion (e.g., about an octant) is consistent with that treatment although in solid state physics, the periodic boundary conditions are used for application to transport properties and to extend the discussion to the band model (which is necessary for understanding band gaps and properties of systems other than conductors, which the free electron model fails to do). The first section, which focuses on the Fermi energy, density of states, and total electronic energy of a free electron gas at absolute zero temperature, was administered in one class period. The second section focusing on the FD and BE distribution functions and their limiting behavior was administered in another class period. Unless specified otherwise, students were instructed to assume that the symbol for momentum $\hbar k$ signifies the magnitude of the momentum vector.

We note that the CQS was implemented with peer interaction [36-41] in the upper-level undergraduate QM class after traditional lecture-based instruction in relevant concepts on the Fermi energy, density of states, and total electronic energy of a solid within the free electron gas model and after learning about the Fermi-Dirac distribution function in the same QM course. When students engaged with the CQS in one-on-one interviews, there was no peer discussion, which may be detrimental [36-42], but the fact that students were asked to think-aloud [35] to make their thought processes clear to the interviewer may have served a somewhat similar purpose. Prior to engaging with the CQS, students took the pretest after traditional lecture-based instruction. After engaging with the CQS, they took the posttest. The five questions on the pretest and posttest focusing on the topics of Fermi energy, density of states, total electronic energy, and distribution functions are the same and they are given in Figure 5.1. In the individual interviews, students answered all five pre/posttest questions together before and after engaging with both sections of the CQS. However, in the written pretest in the undergraduate QM course, students were given the first two questions of the test together in a pretest part I after students learned about the Fermi energy, density of states and total electronic energy of the free electron gas via lecture and questions 3-5 together in another pretest (part II of the pretest) on a different day after students learned about the distribution functions via lecture-based instruction. The posttest was also administered in two parts on two days after students engaged with both sections of the CQS focusing on these concepts and questions 1,4 and 5 were deliberately administered together on one day (part I of the posttest) and questions 2 and 3 were administered together on another day (part II of the posttest). Students had sufficient time to answer the questions on the pre/posttests. We note that since questions 1 and 2 on the test are related (question 1 asks about the Fermi energy and total electronic energy as a conceptual question whereas question 2 asks about them as a question focused on mathematical manipulation) and questions 3-5 are related (question 3 seeks requisite mathematical expressions for the distribution functions and constraints on the number of particles in each single-particle state whereas question 5 asks about the Fermi-Dirac distribution function in graphical representation at two different temperatures and question 4 asks about a limiting case of the quantum distribution functions), the grouping of the questions on the two parts of the *pretest* may have made it easier for the students to answer them in that the related questions in each part of the pretest can prime students to answer the questions more easily than on the *posttest* in which the different types of questions on Fermi energy, total electronic energy and Fermi-Dirac distribution function were deliberately mixed in parts I and II. For example, on pretest part I, if students answered question 2 correctly and found that the Fermi energy does not scale with the size of the system but the total electronic energy does, they can potentially use those results to answer the conceptual question 1 correctly. Similarly, on pretest part II, a student who wrote the correct expression for the Fermi-Dirac distribution function when explicitly prompted in question 3 can potentially take advantage of it to come up with its correct graphical representation in question 5 or find the correct limiting case in question 4. However, as we will see in the results section, student performance on all questions was poor on the pretest after traditional lecture-based instruction, and they did not benefit on the pretest from having similar questions grouped together.

(1) *On your desk, you have two cubes A and B which have N and 2N copper atoms, respectively.*

a. *At temperature $T = 0\ K$, which cube has the higher Fermi energy? Explain your reasoning.*

b. *At temperature $T = 0\ K$, which cube has the higher total electronic energy? Explain your reasoning.*

(2) *Consider a system of N non-interacting electrons in a* ***two-dimensional*** *infinite square well of area A. Let σ be the number of free electrons per unit area and m be the mass of an electron. Using this information, do the following:*

a. *Calculate the Fermi energy for the system.*

b. *Derive an expression for the density of states.*

c. *Calculate the total electronic energy for the system.*

(3) *Give an expression for each of the following distribution functions and give the constraints on each of these distribution functions in terms of how many particles each single-particle state can accommodate.*

a. *Maxwell-Boltzmann:* $n_{MB}(\epsilon) =$

b. *Fermi-Dirac:* $n_{FD}(\epsilon) =$

c. *Bose-Einstein:* $n_{BE}(\epsilon) =$

(4) *Describe the limit in which both the Fermi-Dirac and Bose-Einstein distribution functions approach the Maxwell-Boltzmann distribution function. Explain your reasoning.*

(5) *For a system of identical fermions, using the axes provided, graph the relationship between the distribution function $n_{FD}(\epsilon)$ and energy ϵ for both $T = 0\ K$ and $T > 0\ K$. Be sure to label the Fermi energy. [Note: Students were provided the axes. Also, in the interviews, students were asked about how the distribution function would change when the temperature changes from one non-zero value to another, e.g., $k_B T \gg E_F$.]*

Figure 5.1 Questions students were asked in pre/posttests

These questions map onto the learning goals of the CQS with varying levels of transfer of learning required as follows. In the T = 0 K case, question 1 is a near transfer question directly related to CQ10. Question 2, which relates to CQ1 – CQ7, requires further transfer because the system is two dimensional instead of the three-dimensional system under consideration in CQ1-CQ7. Note that CQ11 was not administered to students, but would offer greater guidance and support to help students answer pre/posttest questions related to two dimensional free-electron gas. For the T > 0 K case, question 3 is a near transfer from CQ12-CQ15 and the subsequent class discussion, and question 4 is a near transfer from CQ14. Finally, question 5 is not a near transfer of the FD distribution function related concepts in questions CQ12-15 (although they have related concepts), since question 5 in the pre/posttest asks students to use a different representation of knowledge. In particular, students have to use graphical representation to answer question 5. Converting from mathematical representation to graphical representation is not easy for students who are still developing expertise in these topics. We note that direct scaffolding pertaining to graphical representation of the FD distribution function can be provided by instructors after the CQS (this is a suggested topic of class discussion following CQ17). We again emphasize that the learning goals of some clicker questions provided in the appendix are not addressed by these test questions. These clicker questions were provided to give a complete picture of the CQS and offer more of the context in which these topics were being discussed.

5.3 RESULTS

A rubric was developed for grading student performance on the five questions on the pretest and posttest. Two of the authors graded all student responses and the inter-grader reliability was better than 95%. Table 5.1 compares the in-class pre/posttest performances of students in upper-level undergraduate QM after traditional lecture-based instruction (pretest) and after they had engaged with the CQS on these concepts (posttest). Tables 1 also presents the normalized gain (g) which is calculated as $g = (post\% - pre\%)/(100\% - pre\%)$ [43]. Moreover, Table 5.1 displays the effect size on each question between the pre/posttest scores, which was calculated as Cohen's $d = (\mu_{post} - \mu_{pre})/\sigma_{pooled}$ where μ_i is the mean of group i and the pooled standard deviation is $\sigma_{pooled} = \sqrt{(\sigma_{pre}{}^2 + \sigma_{post}{}^2)/2}$ [43]. Table 5.1 shows that student performance after traditional lecture-based instruction was poor on all questions. After engaging the CQS, although the average performance improved, it was still at approximately 50% on many of the questions. Below, we discuss student difficulties without separating them into pre/posttest since the difficulties were similar after traditional lecture-based instruction and after students engaged with the CQS, although the difficulties were less prevalent after engaging with the CQS (see Table 5.1).

Table 5.1 Comparison of the mean pre/posttest scores on each question, normalized gains and effect sizes for students in upper-level undergraduate QM (number of students N=13). The pretest was administered after traditional lecture-based instruction and the posttest after students engaged with the entire CQS on these concepts. The percentages in parentheses for questions 1 and 4 refer to the mean scores when students were not graded for whether the reasoning they provided was correct.

Question	Pretest Mean	Posttest Mean	Normalized Gain (g)	Effect Size (d)
1a	8% (8%)	46% (46%)	0.42	0.46
1b	50% (62%)	58% (77%)	0.15	0.09
2a	15%	77%	0.73	1.91
2b	8%	54%	0.50	1.23
2c	8%	50%	0.46	1.33
3	50%	82%	0.64	0.96
4	29% (33%)	50% (62%)	0.29	0.45
5	38%	85%	0.75	1.36

5.3.1 Student difficulties with the Fermi energy

In question 1, many students had difficulty with the fact that the Fermi energy of copper is an intrinsic property and provided responses such as the following: "*Cube B has higher Fermi energy because higher states must be filled*", "*The cube with 2N copper atoms because it has a higher free electron density*", "*B has more atoms, thus it encloses a larger surface area in k-spa*ce". One interviewed student, when asked what the Fermi energy is, stated "[It's] *something to do with exclusion principle. An atom with 10 electrons will settle down to the 10 lowest states.* [There's a] *higher Fermi energy with 20 because there are more being pushed up the ladder with higher energy. An additional one will have additional energy*." This type of reasoning demonstrates either incomplete conceptual understanding of Fermi energy, specifically how the closer level spacing leaves the Fermi energy unchanged. It misses the fact that the volume occupied by each state in the k-space has inverse dependence on the volume of the solid, thus the Fermi energy is an intrinsic property of a given material. Many students also had difficulty differentiating between the Fermi energy and total electronic energy and characterized the Fermi energy as the total energy of all the fermions in the system. Responding to question 1a on the posttest in class, none of the students who answered correctly explicitly derived a mathematical expression for the Fermi energy. However, Figure 5.2 shows the response of a student who answered this conceptual question incorrectly and attempted to derive an expression for the Fermi energy. Unlike many of the other students who struggled to derive the expression for the Fermi energy in response to question 1 a, Figure 5.2 shows that this student wrote down correct equations for the Fermi energy. However, the student incorrectly inferred that the Fermi energy does depend on the number of copper atoms because he did not take into account the volume and the fact that the Fermi energy depends on the number density of the free electrons, which is constant for copper (and not the number of copper atoms). Response to question 2 a in Table 5.1 shows that a majority of students struggled to derive an expression for the Fermi energy after traditional lecture-based instruction but their performance improved significantly after engaging with the CQS.

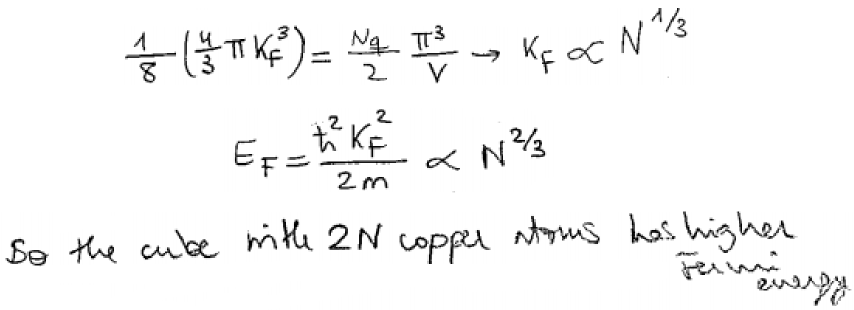


Figure 5.2 A sample response to question 1a in which the student made an incorrect inference "So the cube with 2N copper atoms has higher Fermi energy" based upon his derivation of an expression for the Fermi energy. The student wrote down the equations correctly but did not take into account the volume and the fact that the Fermi energy depends on the number density of the free electrons which is independent of the size of the copper sample.

5.3.2 Student difficulties with the density of states

Many students struggled with the density of states in question 2b with responses such as "$D(\epsilon) = \frac{N}{\frac{\pi k^3}{3}}$" and "$D(\epsilon)$=N/$\epsilon$". When asked to explain what the density of states means, a common difficulty was assuming that it is related to particle number density or probability of occupying a particular single-particle state (confusion between the density of states and the distribution function) as in the following responses: "*This is the number of particles for each energy per k-space volume", "number of particles in each single-particle state with energy ϵ", "the density of particles in a particular energy state", "In a configuration, how close the **occupied** states are to one another", "Particles having energy ϵ per volume".*

5.3.3 Student difficulties with the total electronic energy

In response to question 1b, the most common difficulty was assuming that the total electronic energy would be the same regardless of the number of copper atoms. Discussions suggest that some of them may have been confused because of the fact that the total electronic energy ***per electron*** for a free electron gas is $\left(\frac{3}{5}\right)E_F$ and they remembered it incorrectly as $E_{tot} = \left(\frac{3}{5}\right)E_F$. Moreover, in written responses, two students incorrectly claimed that the copper cube with larger *N* will have a lower total electronic energy since the degeneracy pressure in the larger system would be lower due to its larger dimension. The calculation of the total electronic energy in question 2c was extremely difficult for most students because this calculation cannot be done correctly using an algorithmic approach unlike, e.g., the calculations involving traditional circuit problems in introductory physics in which Kirchhoff's rules can be used algorithmically to yield the correct value of current, voltage and resistance in different parts of a complicated circuit without a functional understanding of the underlying concepts. A majority of students struggled to piece together a solution for the total electronic energy. In an interview, before engaging with the CQS, in response to question 2c in the pretest, one student stated, "*I assume I should integrate but I'm not sure how to set it up.*" The following are typical incorrect responses that suggest that different students struggled with different aspects of setting up the integral: "$E = \int_0^{k_F} E_F dk$", "$E_{tot} = \int_0^{k_F} N d\epsilon$", "$E_{tot} = \int D(\epsilon) d\epsilon$", "$E_{tot} = \int_0^{k_F} D(\epsilon) d\epsilon$", "$E = \int_0^{k_{max}} \frac{\hbar^2 k^2}{2m} dk = \frac{\hbar^2 k_{max}^3}{6m}$", "$E = \int_0^{k_F} \frac{\hbar^2 k^2}{2m} \sigma l_x l_y dk = \frac{\hbar^2 k_{max}^3}{6m}$, *$l_x$ is length of square in x, l_y is length of square in y, σ is number of free electrons per unit area*". Table 5.1 shows that the average student scores on questions 2b and 2c related to the calculation of the density of states and total electronic energy improved from less than 10% after traditional lecture-based instruction to approximately 50% after the CQS. Deriving these expressions was extremely challenging for many students despite the fact that the only difference between the CQS and the pre/posttest questions 2b and 2c is that the dimensionality of the system was two dimensions, rather than three dimensions. Some interviewed students needed guidance from the interviewer to successfully calculate the total electronic energy in question 2c even on the posttest. Other interviewed students (not included in Table 5.1) asked to review CQ1-CQ7 again, which were in the three-dimensional context, before answering question 2c in two dimensions on the posttest.

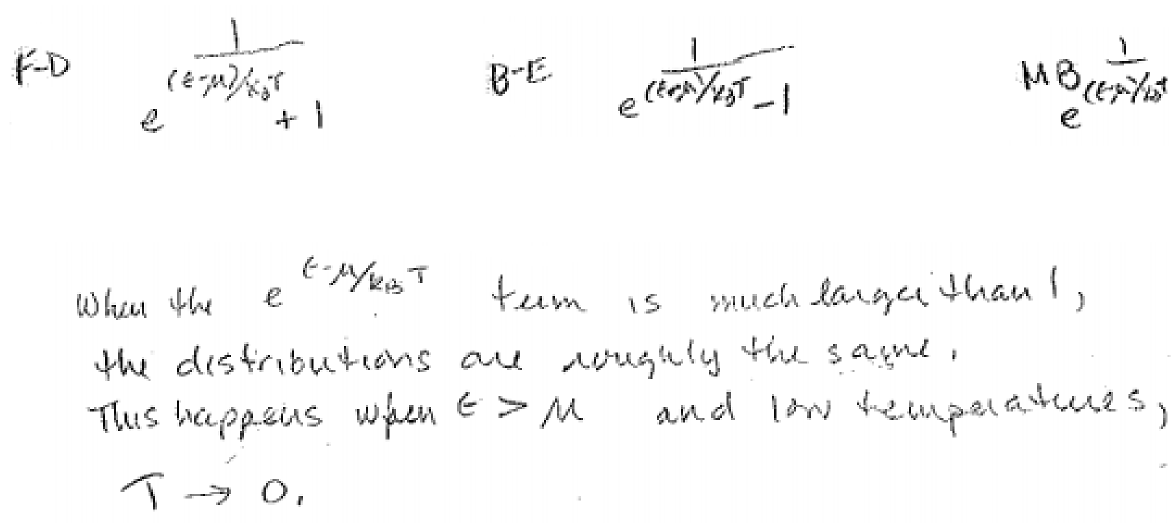
5.3.4 Student difficulties with the expressions for the distribution functions and constraints on the number of particles in each single-particle state

Table 5.1 shows that out of all of the questions, students performed relatively well on both pre/posttests on question 3 which asked for the expressions for the distribution functions and constraints on the number of particles in each single-particle state. On the pretest, average student scores were 39% on the distribution functions and 61% on the constraints and on the posttest, average student scores were 85% on the distribution functions and 80% on the constraints. The most common difficulties with regard to the distribution function was not including the chemical potential in the expressions or interchanging the signs in the denominator for the fermionic and bosonic cases. The most common difficulty for the constraints was switching the fermionic and bosonic cases. Other incorrect responses include claims that the constraint on the number of particles in each single particle state for the fermionic case is between ½ to 1 particle or that it is either 0 or 1 depending on spin. One student stated that for the MB distribution, there is a maximum of one particle in each single-particle state, confusing it with the fermionic case.

5.3.5 Student difficulties with the high temperature limiting case of distribution functions

In the high temperature limit $T \to \infty$, the de Broglie wavelength of the particle wave becomes very small and the overlap of the wavefunction of different particles in the system becomes negligible. In this limit, the Fermi-Dirac and Bose-Einstein distribution functions approach the Maxwell-Boltzmann distribution function. Students had great difficulty with question 4 which focused on this issue (see Table 5.1). The common student difficulties on this question can be classified in a few categories as follows.

Some students claimed that the quantum distribution functions will approach the MB distribution function when $T \to 0\ K$ (which is the exact opposite case in which the quantum effects are important). These students often focused on the mathematical expressions for the quantum distribution functions and mathematically reasoned about how they might approach the MB distribution function. Interviews suggest that students with these types of responses who resorted to using mathematical expressions as the basis for their answer did not think physically about whether their mathematical reasoning made sense conceptually. This dichotomy of either being in the "math" mode (which was prevalent for students who claimed the correct limit was $T \to 0\ K$) or the "physics" mode and not integrating the mathematical and physical reasoning to do the sense-making is a common novice-like problem solving approach and has been observed in other contexts [36]. Two typical responses in this category are: "*When* $T \to 0$, $\frac{1}{e^{\frac{\epsilon-\mu}{k_BT}} \pm 1} \sim \frac{1}{e^{\frac{\epsilon-\mu}{k_BT}}}$", and "*They approach Maxwell-Boltzmann distribution when the exponential part is the most important, so when* $T \to 0$". Figure 5.3 shows another student response that falls in this category. Figure 5.3 shows that the student writes the correct distribution functions in response to question 2 and states in response to question 4 that "*When the* $e^{\frac{\epsilon-\mu}{k_BT}}$ *term is much larger than 1, the distributions are* *roughly the same. This happens when $\epsilon > \mu$ and low temperatures $T \to 0$.*" This response is interesting because the student explicitly notes that the exponential term $e^{\frac{\epsilon-\mu}{k_B T}}$ is much larger than 1 when $\epsilon > \mu$ and $T \to 0$ K but does not contemplate the case when $\epsilon < \mu$ and $T \to 0\ K$. For a fermionic system, this latter case ($\epsilon < \mu$ and $T \to 0\ K$) yields $n_{FD}(\epsilon) = 1$ for all states below the Fermi energy (which is the chemical potential at $T = 0$ K). This type of response suggests that focusing only on mathematical reasoning prevented students from realizing that their reasoning did not take into account all situations (e.g., $\epsilon < \mu$ and $T \to 0$ K in Figure 5.3). Interviews also suggest that some of the students had inadequate understanding of the chemical potential of the system which exacerbated the difficulty in reasoning about the limiting case. For example, students did not realize that μ for particles with mass depends on temperature and for fermions, μ is equal to the Fermi energy at $T = 0$ K and then it decreases with an increase in temperature and eventually becomes negative at high temperatures (while for bosons, μ is zero at and below the critical temperature and is negative otherwise).



F-D $\frac{1}{e^{(\epsilon-\mu)/k_BT}+1}$ B-E $\frac{1}{e^{(\epsilon-\mu)/k_BT}-1}$ MB $\frac{1}{e^{(\epsilon-\mu)/k_BT}}$

When the $e^{\epsilon-\mu/k_BT}$ term is much larger than 1, the distributions are roughly the same, This happens when $\epsilon > \mu$ and low temperatures, $T \to 0$.

Figure 5.3 A sample response in which the student wrote the correct mathematical expressions for each of the distribution functions but drew an incorrect conclusion about the limiting case.

Other students who mainly reasoned using the expression for the distribution functions focused only on large energy ϵ in the expression for the distribution functions, which does not make sense. They claimed that the quantum distribution functions will approach MB distribution function when $\epsilon \to \infty$ as in the following student responses: "*At very large* ϵ, $\frac{\epsilon-\mu}{k_B T} >> 1$ *so it approaches M-B distribution*", "*As* $\epsilon \to \infty$, *all converge b/c the* ± 1 *in denominator becomes irrelevant*", "*In the high* ϵ*-limit, as the exponential term becomes very large*".

Other students claimed that the quantum distribution functions will approach the MD distribution function whenever the particles are non-interacting, as in the following responses: "*If there is no interaction, both of them* [Fermi-Dirac and Bose-Einstein] *become classical* [Maxwell-Boltzmann]"or "*If there is no interaction…classical.*" Discussions suggest that these students often confused the fact that the overlap of the wavefunction of different particles in the system should be negligible (which happens in the high temperature limit) to conclude that the particles should be non-interacting or Coulomb interaction between the electrons should be negligible to approach the MB distribution limit.

5.3.6 In-class implementation by instructor A

The ability to transform from one representation of knowledge to another, e.g., mathematical to graphical, is a sign of expertise. Experts often transform from one representation of knowledge to another to simplify the problem solving process. Table 5.1 shows that on question 5 on the pre/posttests that asked students to draw the Fermi-Dirac distribution function at *T=0 K* and *T > 0 K* students' average score more than doubled after engaging with the CQS following traditional lecture-based instruction. On the pretest, many students struggled with the graphical representation of the Fermi-Dirac distribution function both at zero and non-zero temperatures. For example, Figure 5.4 shows one such graph on which an interviewed student drew an exponentially increasing $n_{FD}(\epsilon)$ vs. ϵ at $T > 0\ K$.

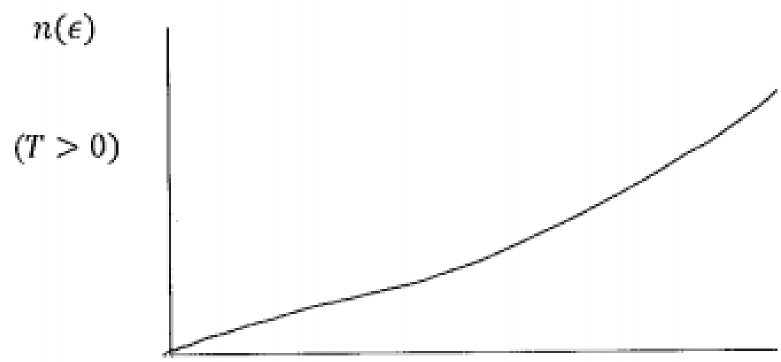


Figure 5.4 An interviewed student's incorrect graphical representation of the Fermi-Dirac distribution function at T > 0K stating the graph has exponential shape because the expression for $\mathbf{n_{FD}}(\boldsymbol{\epsilon})$ involves "…e to the something… probably has energy in there. I'm not so sure just how temperature would fit into it though."

Another interviewed student incorrectly claimed that as the temperature increases, a peak appears in $n_{FD}(\epsilon)$ and that peak in the Fermi-Dirac distribution function would shift to higher temperatures and the occupation of the ground state would eventually reach zero (see his drawing in Figure 5). "*For T>0, there's a local maximum at ϵ=0, but it gets pushed out as T increases. Much, much greater, and it would get pushed out past the Fermi energy. I wouldn't think there should be anything keeping that maximum at the Fermi energy*." Interviews suggest that some students may have been confused about the peak in the Maxwell speed distribution (which has the square of the speed from the volume element multiplying the exponential factor so that there is a peak at a non-zero value of speed) and how the peak in that distribution moves to higher energies as the temperature increases. In written responses to question 5 also, several students drew the

Fermi-Dirac distribution function with peaks at the Fermi energy or some other non-zero energy similar to Figure 5.5. For example, one student who drew the Fermi-Dirac distribution function correctly at $T=0\ K$, drew a graph similar to that shown in Figure 5.5 for $T >>0\ K$. Another student drew a graph similar to that shown in Figure 5.5 for $T >>0\ K$ for both $T=0\ K$ and $T > 0\ K$ with peaks of different heights centered at the same value of single-particle energy. Other students who confused the fermionic and bosonic distribution functions, drew the Fermi-Dirac distribution function to be a delta function at $\epsilon = 0$ at $T = 0\ K$.

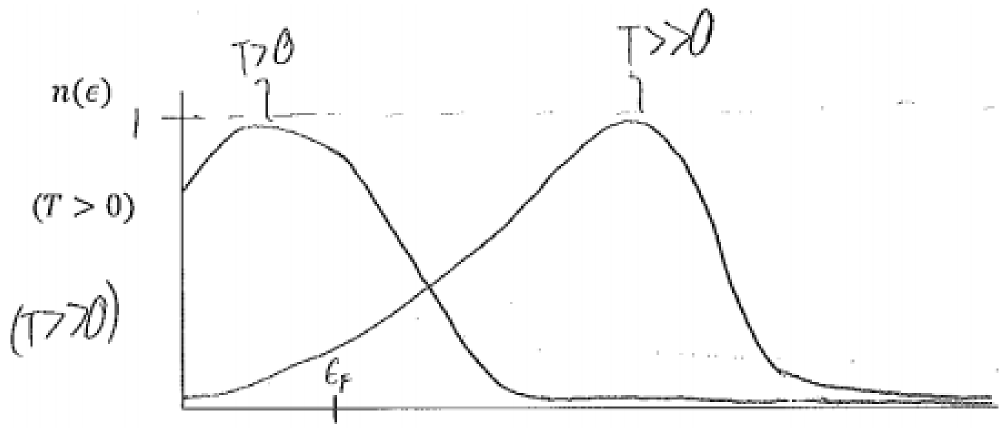


Figure 5.5 An interviewed student's incorrect graphical representation of the Fermi-Dirac distribution function in which the student incorrectly stated that the single-particle ground state of the fermions would eventually be vacated and the peak in the distribution function (which is not supposed to be there) will keep shifting to higher energies as the temperature of the system increased.

5.4 SUMMARY AND FUTURE PLANS

We investigated the difficulties that physics students in upper-level undergraduate QM and graduate students after quantum and statistical mechanics core courses have with the Fermi energy, Fermi-Dirac distribution and total electronic energy of a free electron gas after they had learned relevant concepts in their respective courses. These difficulties were probed by administering written conceptual and quantitative questions to undergraduate students and asking students in undergraduate and graduate courses to answer those questions while thinking aloud [35] in one-on-one individual interviews. We find that advanced students have many common difficulties with these concepts, after traditional lecture-based instruction and students struggled with both conceptual and quantitative questions. We also find that student performance in the undergraduate course improved after students engaged with the CQS on relevant concepts but there is still substantial room for improvement.

The future refinements of the CQS will focus on addressing student difficulties found via in-class administration (in-vivo) as opposed to via the earlier administration in the one-on-one interview situation (in-vitro). For example, in order to better address the difficulties with the distribution function, an increased emphasis on the chemical potential, its role in the distribution functions, and its behavior as a function of temperature will be included in the CQS via additional clicker questions. The common difficulties with the limiting case posed in question 4 will also be addressed more explicitly via additional clicker questions. Moreover, although it is typical to guide students through calculational problems (that involve both conceptual and quantitative parts) via a series of clicker questions as in CQ1-CQ7, student learning may be improved for question 2 which involves calculations of the Fermi energy, density of states and total electronic energy by changing the implementation of the CQS. In fact, a majority of interviewed students required at least some guidance from the interviewer via leading questions in order to do the calculations correctly in question 2 on the posttest, which focused on a two dimensional system instead of the three dimensional system treated in CQ1-CQ7. Some interviewees asked to review CQ1-CQ7 one more time for the three dimensional calculations before calculating the corresponding quantities in two dimensions in question 2 on the posttest. In the future implementation of the CQS, immediately after the students engage with clicker questions CQ1-CQ7 in the class, we plan to ask them to respond to question 2 without any support so that they have an opportunity to reflect upon their proficiency in deriving the expressions for the Fermi energy, density of states and total electronic energy of a free electron gas and tell them right before they engage with the CQS that they will have to do the derivations immediately after the CQS as a quiz. This type of immediate individual reflection after engaging with the CQS with their peers may be helpful in improving individual accountability and focus, and help students consolidate the concepts learned and develop facility and self-reliance in calculating these quantities by combining conceptual and quantitative problem solving.

5.5 ACKNOWLEDGEMENTS

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5.7 CHAPTER APPENDIX

*Notation and procedures coincide with treatment by Griffiths (2nd Edition). Correct answers are **bolded.***

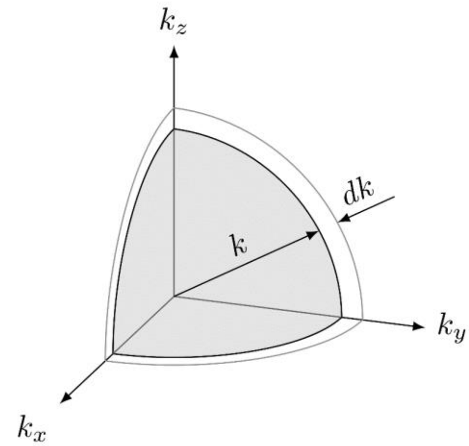

Figure 5.6 Illustration provided to students with the CQ1-CQ10 (Credit: Kyle Whitcomb, University of Pittsburgh)

Section 1 (T = 0 K):

(CQ1) *Let's consider an octant in k-space. Choose all of the following statements that are correct about the k-space for a free electron gas at T = 0 K in a three-dimensional solid volume V made up of N atoms each with q free electrons, given that two electrons with opposite spins occupy a volume* $\frac{\pi^3}{V}$ *in k-space.*

(1) *In k-space, the volume of an octant with highest occupied wavevector* k_F *is* $\frac{1}{8}(volume\ of\ sphere\ with\ radius\ k_F) = \frac{1}{8}\left(\frac{4}{3}\pi k_F^3\right) = \left(\frac{1}{6}\pi k_F^3\right)$.

(2) *The total volume occupied by the free electrons is* $\frac{(Total\ number\ of\ free\ electrons)}{2}$ *(Volume occupied by two electrons in k-space)* $= \frac{Nq}{2}\left(\frac{\pi^3}{V}\right)$.

(3) *The volume of an octant with highest occupied wavevector* k_F *and the total volume occupied by the free electrons in k-space are equal, so* $\left(\frac{1}{6}\pi k_F^3\right) = \frac{Nq}{2}\left(\frac{\pi^3}{V}\right)$.

*A. 1 only   B. 2 only   C. 1 and 2 only   D. 2 and 3 only   **E**. all of the above*

(CQ2) *Equating* $\left(\frac{1}{6}\pi k_F^3\right) = \frac{Nq}{2}\left(\frac{\pi^3}{V}\right)$ *and solving for* k_F *gives* $k_F = (3\pi^2\rho)^{1/3}$ *where* $\rho = \frac{Nq}{V}$ *is the free electron density (number of free electrons per unit volume). Using this information, choose all of the following statements that are correct about the Fermi energy* E_F *for non-interacting electrons in the free electron gas model.*

1) *The Fermi energy* E_F *is the energy of the highest occupied state at* $T = 0\ K$.
2) *The Fermi energy is* $E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}(3\pi^2\rho)^{2/3}$
3) *The Fermi energy* E_F *only depends on the electron number density and the mass of the electron.*

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only ***E****. all of the above*

(CQ3) *Choose all of the following statements that are correct about a free electron gas* <u>*in three dimensions*</u>.

1) *Each state in each shell between k and k+dk has energy* $\epsilon = \frac{\hbar^2 k^2}{2m}$.
2) *The volume of a shell of thickness* dk *between k and k+dk in the relevant octant in k space occupied by free electrons is* $\frac{1}{8}\left(\frac{4}{3}\pi k^3\right)dk$.
3) *The volume of a shell of thickness* dk *between k and k+dk in the relevant octant in k space occupied by free electrons is* $\frac{1}{8}(4\pi k^2)dk$.

A. 2 only B. 3 only C. 1 and 2 only ***D****. 1 and 3 only E. None of the above.*

(CQ4) *Choose all of the following statements that are correct for the 3D free electron gas model. (Include electron spin when relevant.)*

1) *The number of electron states in each shell between k and k+dk is:*

$$\frac{2\ x\ Volume\ of\ Shell}{Volume\ associated\ with\ a\ single\ state\ in\ k{-}space} = \frac{2\cdot\frac{1}{8}(4\pi k^2)dk}{\frac{\pi^3}{V}} = \frac{V}{\pi^2}k^2 dk.$$

2) *The total energy of the electrons in a shell between k and* $k + dk$ *is* $\frac{\hbar^2 k^2}{2m}\frac{V}{\pi^2}k^2 dk$ *where* $\epsilon = \frac{\hbar^2 k^2}{2m}$.
3) *The total electronic energy of the system at T = 0 K can be calculated as:*
$$E_{tot} = \int_0^{k_F}\frac{\hbar^2 k^2}{2m}\frac{V}{\pi^2}k^2 dk = \frac{\hbar^2}{2m}\frac{V}{\pi^2}\int_0^{k_F}k^4 dk = \frac{\hbar^2}{2m}\frac{V}{\pi^2}\frac{k_F{}^5}{5}$$

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only ***E****. All of the above.*

(CQ5) *Choose all of the following statements that are correct about a free electron gas* *in three dimensions*. *(Include electron spin when relevant. ϵ defines a surface in k-space. A shell is the volume between two closely-spaced energy surfaces.)*

1) The number of states in each shell between ϵ and $\epsilon+d\epsilon$ is $D(\epsilon)\, d\epsilon$ where the density of states, $D(\epsilon)$, is the number of states per small interval of energy for a given ϵ.
2) The density of states, $D(\epsilon)$, is the number of particles in a given energy interval between energy ϵ and $\epsilon+d\epsilon$.
3) For a free electron gas at T = 0 K, the total energy, E_{tot}, can be calculated as $E_{tot} = \int_0^{E_F} \epsilon\, D(\epsilon) d\epsilon$

A. 1 only B. 1 and 2 only ***C****. 1 and 3 only D. 2 and 3 only E. All of the above.*

(CQ6) *Consider the following conversation:*

Student 1: "For a free electron gas at T = 0 K, the total electronic energy $E_{tot} = \int_0^{E_F} D(\epsilon) d\epsilon$."
Student 2: "I disagree. Your integral gives the total number of states *up to the Fermi energy."*
Student 3: "The total energy is $E_{tot} = \int_0^{E_F} \epsilon\, D(\epsilon) d\epsilon$, which can also be calculated in terms of k as we did in a preceding question."

A. Student 1 only B. Student 2 only C. Students 1 and 3 only ***D****. Students 2 and 3 only E. All of the above.*

(CQ7) *Choose all of the following statements that are correct about the density of states, $D(\epsilon)$, for the* ***3D free electron gas model*** *given that the number of electron states in the shell between k and k+dk is $\frac{V}{\pi^2} k^2 dk$ (electron spin has been included).*

1) $D(\epsilon) d\epsilon = \frac{V}{\pi^2} k^2 dk$. Therefore, $D(\epsilon) d\epsilon$ is proportional to $k^2 dk$.
2) Given that $\epsilon = \frac{\hbar^2 k^2}{2m}$, $d\epsilon = \frac{\hbar^2}{m} k dk$.

3) Using (1) and (2), $D(\epsilon) d\epsilon$ is proportional to $\sqrt{\epsilon} d\epsilon$. Therefore $D(\epsilon)$ is proportional to $\sqrt{\epsilon}$.

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only ***E****. All of the above.*

(CQ8) *We now know that the total electronic energy of the system of free electrons at $T = 0K$ is* $E_{tot} = \left(\frac{\hbar^2 (3\pi^2 Nq)^{5/3}}{10\pi^2 m}\right) V^{-2/3}$ *, which can be written as a function of volume given that the number of free electrons is fixed:* $E_{tot} = C\,V^{-2/3}$*. Then* $dE_{tot} = (-2/3)C\,V^{-5/3}dV$*.*

Choose all of the following that are correct. (Assume no heat transfer from the free electron gas to its surroundings in the process discussed below).

1) *If dV is negative, dE_{tot} is positive.*
2) *The infinitesimal work by the system $dW = PdV = -dE_{tot}$, so the "degeneracy pressure" $p = (\frac{2}{3})C\,V^{-5/3}$.*
3) *The degeneracy pressure is due to the anti-symmetrization requirement of the many-particle wavefunction of the electrons.*
4) *Since decreasing the volume of the system increases the energy, it is not energetically favorable.*

A. 1 and 2 only B. 1 and 3 only C. 2 and 3 only D. 1, 2, and 3 only

***E**. All of the above.*

(CQ9) *Choose all of the following statements that are correct about a free electron gas system.*

1) *"Degeneracy pressure" describes the quantum mechanical effect that there is an "outward" force per unit area that prevents a solid from collapsing due to the restriction that each electron must occupy a different single particle state.*
2) *The degeneracy pressure plays a role in stabilizing a solid object.*
3) *If the electrons were bosons, the total electronic energy of the free electron gas at temperature T = 0K would be lower than what it actually is.*

*A. 1 only B. 3 only C. 1 and 2 only D. 1 and 3 only **E**. All of the above.*

(CQ10) *Cubes A and B with the same atom number density have N and 2N sodium atoms, respectively. Choose all of the following statements that are correct.*

1) *At temperature T = 0 K, the Fermi energy of sodium in cube B is larger than the Fermi energy of sodium in cube A.*
2) *At temperature T = 0 K, the total electronic energy of the electrons in cube B is larger than the total electronic energy of the electrons in cube A.*
3) *If we slowly compress the volume of cube A, the total electronic energy of the electrons in cube A will increase.*

A. 1 only B. 2 only C. 1 and 2 only ***D.*** *2 and 3 only E. All of the above.*

Class Discussion (3D free electron gas at T = 0 K)

- *Two electrons in the same spatial state with "opposing" spins occupy a volume* $\frac{\pi^3}{V}$ *in* k*-space (regardless of the value of* $\vec{k}$*).*
- *The volume* $\frac{\pi^3}{V}$ *in* k*-space can accommodate two electrons due to the fact that electrons are spin-1/2 fermions.*
- *For an octant, the volume of a shell between k and k+dk of thickness* dk *is* $\frac{1}{8}(4\pi k^2)dk$.
- *The number of electron states in the shell between k and k+dk is* $\frac{V}{\pi^2}k^2dk$, *which is equal to* $D(\epsilon)d\epsilon$ *where* $D(\epsilon)$ *is the density of states with* $\epsilon = \frac{\hbar^2k^2}{2m}$.
- *The energy of the electrons in a shell of thickness* dk *is* $dE = \frac{\hbar^2k^2}{2m}\frac{V}{\pi^2}k^2dk$.
- *The total electronic energy is* $E_{tot} = \frac{\hbar^2}{2m}\frac{V}{\pi^2}\int_0^{k_F}k^4dk = \frac{\hbar^2}{2m}\frac{V}{\pi^2}\frac{{k_F}^5}{5} = \left(\frac{\hbar^2\left(3\pi^2Nq\right)^{5/3}}{10\pi^2m}\right)V^{-2/3}$.
- *"Degeneracy pressure" is an "outward" quantum mechanical force per unit area that prevents the system from collapsing.*

The following question was not administered in this study but could help scaffold transfer from 3D to 2D in future implementations.

(CQ11) *Choose all of the following statements that are correct about the density of states, $D(\epsilon)$, for the* ***2D free electron gas model*** *given that the number of electron states in the shell between k and k+dk is $\frac{A}{\pi}kdk$ (electron spin has been included when relevant).*

1) $D(\epsilon)d\epsilon = \frac{A}{\pi}kdk$. Therefore, $D(\epsilon)d\epsilon$ is proportional to kdk.
2) Given that $\epsilon = \frac{\hbar^2k^2}{2m}$, $d\epsilon = \frac{\hbar^2}{m}kdk$.

3) Using (1) and (2), $D(\epsilon)d\epsilon$ is proportional to $d\epsilon$, therefore $D(\epsilon)$ does not depend on energy ϵ.

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only ***E***. *All of the above.*

Section 2 (System at T > 0 K):

(CQ12)
- *The distribution function $n(\epsilon)$ is the average number of particles in one single particle state with energy ϵ.*
- *For a given system, $D(\epsilon)$, the* ***density of states*** *for energy ϵ, is the number of single particle states per unit energy with energy ϵ.*
- *The average number of particles per unit energy with energy ϵ is $N(\epsilon)$.*

Choose all of the following statements that are correct:

1) $n(\epsilon) = \frac{N(\epsilon)}{D(\epsilon)}$
2) *Fermions, bosons, and distinguishable particles have different $n(\epsilon)$.*
3) *Bosons and distinguishable particles have the same $n(\epsilon)$ because there is no limit to the number of particles that can occupy a given single-particle state, unlike fermions.*

A. 1 only B. 2 only C. 3 only ***D.*** *1 and 2 only E. 1 and 3 only.*

(CQ13) *Choose all of the following statements that are correct about* $n(\epsilon)$ $(all\ symbols\ have\ their\ usual\ meaning)$:

1) *The distribution function* $n(\epsilon)$ *is the average number of particles in a given single-particle state with energy* ϵ.
2) *The distribution function is* $n(\epsilon) = e^{\frac{-(\epsilon-\mu)}{k_B T}}$ *in situations in which the particles can be treated as distinguishable.*
3) $0 \leq n(\epsilon) \leq 1$ *for all single particle states with energy* ϵ *regardless of whether the particles are bosons or fermions.*

A. 2 only B. 3 only ***C.*** *1 and 2 only D. 2 and 3 only E. All of the above.*

Class Discussion

$D(\epsilon)$ - *"Density of states"* - *The number of single particle states per unit energy with energy* ϵ.
$n(\epsilon)$ - *"Distribution Function" – The average number of particles in a given single particle state with energy* ϵ.
$N(\epsilon) = D(\epsilon)n(\epsilon)$ *is the average number of particles per unit energy with energy* ϵ.

Depending on the type of particles, the distribution function $n(\epsilon)$ *can be one of the following:*

- *Maxwell-Boltzmann:* $n(\epsilon) = \frac{1}{e^{\frac{\epsilon-\mu}{k_B T}}}$
- *Fermi-Dirac:* $n(\epsilon) = \frac{1}{e^{\frac{\epsilon-\mu}{k_B T}}+1}$
- *Bose-Einstein:* $n(\epsilon) = \frac{1}{e^{\frac{\epsilon-\mu}{k_B T}}-1}$

Review the differences between <u>*fermions*</u>*,* <u>*bosons*</u>*, and* <u>*distinguishable particles*</u> *with respect to issues discussed in the two prior questions.*

(CQ14) *Choose all of the following statements that are correct about the Maxwell-Boltzmann distribution (MBD),* $n(\epsilon) = \frac{1}{e^{\frac{\epsilon-\mu}{k_B T}}}$.

1) *The Maxwell-Boltzmann distribution can be used for classical distinguishable particles.*
2) *In the expression* $n(\epsilon) = \frac{1}{e^{\frac{\epsilon-\mu}{k_B T}}}$, ϵ *represents the energy of a single-particle state.*
3) *In the high temperature limit, the Fermi-Dirac and Bose-Einstein distribution functions reduce to the MBD* $n(\epsilon) = \frac{1}{e^{\frac{\epsilon-\mu}{k_B T}}}$

A. 1 only B. 2 only C. 1 and 2 only D. 1 and 3 only ***E****. All of the above.*

(CQ15) *Choose all of the following statements that are correct about non-interacting fermions. Recall that the Fermi-Dirac distribution function is* $n(\epsilon) = \frac{1}{e^{\frac{\epsilon-\mu}{k_B T}}+1}$.

1) *At T = 0 K (absolute zero temperature),* $n(\epsilon)$*=1 if* $\epsilon > \mu(T = 0)$ *and* $n(\epsilon)$*=0 if* $\epsilon < \mu(T = 0)$.
2) *At T = 0 K (absolute zero temperature), the Fermi energy is equal to the chemical potential* $\mu(T = 0)$.
3) *At a finite non-zero temperature, if* $\epsilon = \mu(T)$*, the average occupation number for a particular single particle state with energy* ϵ *is* $n(\epsilon) = 1/2$.

A. 1 only B. 1 and 2 only C. 1 and 3 only **D.** *2 and 3 only E. All of the above.*

(CQ16) *Choose all of the following statements that are correct about non-interacting bosons.*

(1) The chemical potential for a bosonic system is always less than or equal to zero, $\mu(T) \leq 0$.

(2) As the temperature decreases, the chemical potential $\mu(T)$ *increases.*

(3) Bose-Einstein condensation can occur at low temperatures when a macroscopic number of bosons occupies the lowest single-particle state or ground state.

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only ***E****. All of the above.*

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*(**CQ17**) Given the distribution function* $n(\epsilon) = \frac{1}{e^{\frac{\epsilon-\mu(T)}{k_B T}}-1}$ *for massive bosons, choose all of the following statements that are true related to the chemical potential of the system:*

1) $n(\epsilon)$ *cannot be negative, so* $\frac{\epsilon-\mu(T)}{k_B T} > 0$.
2) $\epsilon - \mu(T) > 0$ *implies that* $\epsilon > \mu(T)$ *for all allowed single particle energies* ϵ.
3) *Since the lowest single particle energy* $\epsilon \sim 0$, $\epsilon > \mu(T)$ *for all* ϵ *implies that* $\mu(T)$ *for a boson is always negative.*

*A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only **E**. All of the above.*

Class Discussion

Discuss issues pertaining to the preceding questions such as these:

At high temperature, why do the Fermi-Dirac and Bose-Einstein distribution functions both reduce to the Maxwell-Boltzmann distribution function?

What do the graphical representations of the various distribution functions look like at different temperatures?

6.0 IMPACT OF INCOROPORATING MATHEMATICAL RIGOR IN A QUANTUM INTERACTIVE LEARNING TUTORIAL ON STUDENTS' CONCEPTUAL UNDERSTANDING OF QUANTUM OPTICS

6.1 INTRODUCTION

6.1.1 Background on expertise

In order to help students develop expertise in any area of physics, one must first ask how experts, in general, compare to novices in terms of their knowledge structure and their problem-solving, reasoning, and metacognitive skills. According to Sternberg [1], some of the characteristics of an expert in any field include the following: (1) having a large and well organized knowledge structure about the domain; (2) spending significant amount of time in determining how to represent problems before searching for a problem strategy, (i.e., analyzing the problem and planning the solution); (3) developing representations of different problems based on deep underlying structural similarities between problems; (4) working forward from the given information in the problem and implementing strategies to find the unknowns; (5) efficient problem solving—when under time constraints, experts solve problems more quickly than novices; and (6) accurately predicting the difficulty in solving a problem. Additionally, experts are more flexible than novices in their planning and actions [2].

Experts also have more robust meta-cognitive skills than novices. Meta-cognitive skills or self-regulatory skills, refer to a set of activities that can help individuals control their learning [3-5]. The three main self-regulatory skills are planning, monitoring, and evaluation [3-5]. Planning involves selecting appropriate strategies to use before beginning a task. Monitoring is the awareness of comprehension in light of the problem and task performance. Evaluation involves appraising the product of the task and reevaluating conclusions [3-5]. Self-regulatory skills are especially important for learning in knowledge-rich domains such as physics. For example, in physics, students benefit from approaching a problem in a systematic way, such as analyzing the problem (e.g., drawing a diagram, listing knowns and unknowns, and predicting qualitative features of the solution that can be checked later), planning (e.g., selecting pertinent principles or concepts to solve the problem), and evaluating (e.g., checking that the steps are valid and that the answer makes sense) [6-32]. When experts repeatedly practice problems in their domain of expertise, problem-solving and self-regulatory skills may even become automatic and subconscious [3-5]. Therefore, unless experts are given a “novel” problem, they may go through the problem-solving process in an automated manner without making a conscious effort to plan, monitor, or evaluate their work [6]. Although individuals’ expertise in a domain spans a wide spectrum on a continuum, with this caveat in mind, here we refer to physics instructors as experts and students as novices.

If our goal is to help students become experts in physics, whether at the introductory or advanced level, we must also contemplate whether there is something special about the nature of expertise in physics over and above what is true in general about expertise, e.g., what is needed for becoming an expert tennis or chess player or music performer [33-38]. Physics is a discipline that focuses on unraveling the underlying mechanisms of new physical phenomena in our universe. Physicists make and refine models to test and explain physical phenomena that are observed or to predict those that have not been observed so far. A cohesive physical model requires synthesis of both conceptual and quantitative knowledge as shown schematically in Fig. 6.1. Therefore, an important aspect of expertise in physics is the proficiency with which one makes appropriate connections between physics concepts necessary to understand physical phenomena and relevant mathematics. Indeed, in physics, there are very few fundamental laws which are encapsulated in compact mathematical forms and learning to unpack them can help develop expertise and organize one's knowledge hierarchically. In particular, developing expertise in physics entails making appropriate math-physics connection in order to meaningfully unpack, interpret and apply the laws of physics and use this sense-making to develop a good knowledge structure of physics and solve novel problems in diverse situations. It is important to recognize that meaningful sense-making to unpack, interpret and apply the laws of physics, develop and organize one's knowledge structure, and retrieve relevant knowledge to solve complex physics problems is an iterative dynamic process (see Fig. 6.1) and appropriate reflection and meta-cognition during problem solving is required to give individuals an opportunity to refine, repair and extend their knowledge structure and propel them towards a higher level of expertise.

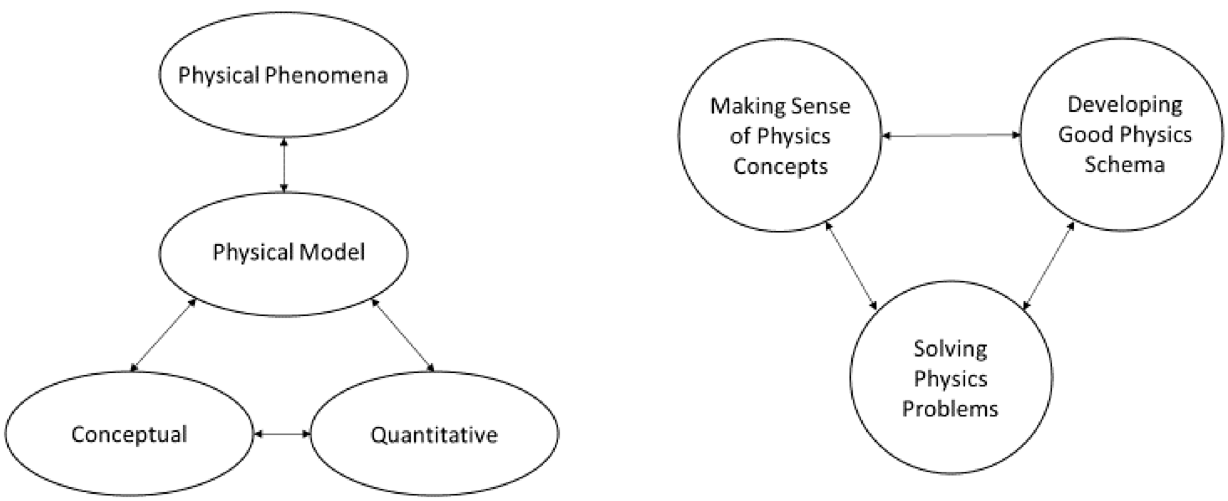


Figure 6.1 Schematic diagram showing connections between physical phenomena and modeling involving integration of conceptual and quantitative understanding in physics (left) and different synergistic components of expertise development in physics (right).

Unfortunately, even though some major goals of physics courses for physics majors (as well as for other science and engineering majors) are to enable students to develop good reasoning and problem solving skills, use these skills in a unified manner to explain, predict diverse physical phenomena in everyday experience, numerous studies show that from a traditionally taught course, many students do not acquire these skills and develop the level of expertise desired [6-32]. The difficulty in physics expertise development and learning to think like a physicist can partly be attributed to the fact that many traditional courses from introductory to advanced level do not focus on helping students master the complex chain of reasoning that is often required to solve problems in the relatively precise domain of physics. Students have difficulty in making the appropriate math-physics connection, which is critical for productive problem solving and using it to develop a robust knowledge structure [6].

6.1.2 ICQUIP framework for developing expertise in physics from introductory to advanced levels

Since appropriate qualitative (conceptual) and quantitative connection and sense-making are central to becoming an expert in physics but are often not adequately recognized and accounted for in traditional physics teaching at all levels for science and engineering majors via serious contemplation of instructional goals, instructional design and assessment of learning, we propose a framework called "Integrating Conceptual and Quantitative Understanding In Physics" or "ICQUIP". This framework focuses on an essential ingredient in physics instruction in order to develop students' expertise adequately and equip them with both conceptual and quantitative knowledge and skills to unpack the laws of physics encapsulated in compact mathematical forms and use physics problem solving for learning and organizing their knowledge hierarchically [6].

The ICQUIP framework asserts that without focus on appropriate integration of conceptual and quantitative understanding in physics, commensurate with students' prior knowledge and skills, physics learning will not be functional. Rather, many students may perform well in their physics courses by memorizing concepts and formulas and solving the problems algorithmically using plug and chug approaches. Indeed, prior research suggests that many students view physics as a collection of disconnected facts and formulas and believe that performing well in physics courses entails memorizing and regurgitating algorithms and doing pattern matching while solving problems [39-41]. The goal of the ICQUIP framework is to draw attention to the nature of expertise in physics and emphasize the central role of the integration of an appropriate level of conceptual and quantitative knowledge and skills and why this integration must be incorporated in instructional goals, design and assessment in order for students at both the introductory and advanced levels to truly become physics experts.

The ICQUIP framework that explicitly brings out the importance of appropriate conceptual and quantitative connection in teaching, learning and assessment for physics expertise development is particularly important because of several related common misconceptions that physics instructors at all levels often have. For example, instructors often believe that learning physics concepts is easier for students at all levels than learning how to solve physics problems using "rigorous" mathematics [42-45]. They believe that if non-science majors can learn physics concepts, science and engineering majors (and particularly physics majors) can learn physics concepts on their own and there is no point in wasting precious instructional time on concepts instead of focusing on mathematical derivations and problems that will help students do complex calculations. Moreover, in upper-level or graduate courses, instructors often believe that students should have learned the concepts in the previous physics courses (e.g., in undergraduate courses for graduate core courses) so their goal as instructors is mainly to focus on developing the "calculational" facility of students in the courses they are teaching instead of striving to appropriately integrate conceptual and quantitative understanding [42]. Some instructors also believe that students will learn the physics concepts anyway in order to be able to do the calculations so there is no need to reward them for conceptual understanding by asking them conceptual questions in assessment tasks [42]. Other instructors claim that they always mention important concepts involved before doing calculational problems or before doing complicated derivations in their classes [42]. However, they only ask students to do complicated calculations in assessment tasks that determine their course grade (these are often problems that many students attempt to do using algorithmic or plug and chug approaches) because this is the most efficient use of instruction and learning time. Also, even if students have had one coat of exposure to concepts in previous courses, integrating conceptual and quantitative aspects of physics in instructional goals, instructional design and assessment of learning is critical for a majority of students to be motivated to focus on functional understanding and be supported to develop a good knowledge structure of physics by solving a variety of integrated problems that are appropriately scaffolded. Some instructors also claim that they select calculational problems that have rich conceptual implications although they expect students to unpack those conceptual implications on their own when doing the calculation instead of explicitly integrating conceptual questions with those calculational problems in order to provide scaffolding support to make appropriate math-physics connections (without such incentive and support, many students at all levels do not make such connections automatically and conceptual learning and development of a robust knowledge structure and skills are compromised).

The ICQUIP framework's explicit focus on appropriate integration of conceptual and quantitative understanding in physics for expertise development is important for instruction because physics is one of those disciplines in which quantitative facility and algorithmic approaches can mask the lack of a robust knowledge structure and deep conceptual understanding. In order to become an expert in physics, students must learn to integrate conceptual and quantitative aspects of physics in a meaningful way and internalize each equation encountered in physics problem solving as a relation between physical quantities, and not merely as a plug-and-chug tool or a "formula" to obtain a solution. However, since traditional physics courses for physics majors (and science and engineering students in general) often focus primarily on quantitative assessments, the algorithmic approaches to solving physics problems that do not reflect conceptual understanding can lead to many students obtaining good grades despite having superficial understanding of the underlying physics concepts and novice-like knowledge structure. Since many students focus on what they are graded on, lack of emphasis on conceptual understanding disincentivizes metacognition and making appropriate math-physics connection to develop a robust knowledge structure. In fact, motivational goal orientation of students can be divided into two broad categories: goal orientation of students who are focused mainly on performing well in a course instead of on developing expertise, i.e., a 'performance' goal orientation, and those who are focused on achieving mastery of the material, i.e., a 'mastery' goal orientation [46–48]. These different motivational goals can have a negative or positive feedback loop effect on student attitudes and may shape their problem-solving beliefs and processes through different levels of engagement and sense-making while solving problems [48]. Unlike expertise in playing tennis or chess or music performance, in which performance goal orientation would be commensurate with the desire for mastery (so that the difference between performance and mastery goals blur), there can often be a huge gulf between performance and mastery goal orientations in traditionally taught physics courses that evaluate student learning mainly on algorithmic problem solving, which can be accomplished using plug and chug approaches. In such courses, many students who are motivated mainly by the course grade are disincentivized to develop mastery and may not make sufficient effort to integrate math and physics appropriately and build a good knowledge structure.

We also note that contrary to the common misconception of physics instructors, conceptual reasoning without using quantitative tools can often be more challenging than reasoning conceptually with quantitative tools, particularly for those who are not experts, because quantitative problems can be solved algorithmically by constraint satisfaction. This is because novices' knowledge hierarchy is fragmented and the limited capacity of working memory makes the cognitive load high during a conceptual reasoning task when no quantitative anchors are available, leaving fewer cognitive resources available for metacognition [49]. On the other hand, research shows that many students in physics courses, who have become facile at quantitative manipulation, are unable to answer similar isomorphic questions posed *conceptuall*y. In other words, if only quantitative problems are posed, students often view them as ``plug-and-chug'' exercises while conceptual problems alone are viewed as guessing tasks with little connection to physics. Indeed, teaching students to draw conceptual inferences from quantitative tools constitutes an important yet under-emphasized tool for helping them learn physics and develop their reasoning and meta-cognitive skills because once students have solved a quantitative problem, the cognitive resources may be freed up for drawing meaningful conceptual inferences. Thus, the ICQUIP framework is important for physics instruction because, without guidance, most students do not exploit quantitative problem solving as an opportunity to reflect upon their answers conceptually and build a good knowledge structure. For example, if a student knows which equations are involved in solving a problem, he or she can combine them in any order to obtain a quantitative answer. On the contrary, while reasoning conceptually without quantitative tools, the student must understand the physics underlying the given situation and generally proceed in a particular order to arrive at the correct conclusion [6]. Therefore, the probability of deviating from the correct reasoning chain increases rapidly as the chain of conceptual reasoning becomes long because most students do not have sufficient level of expertise. Combining quantitative and conceptual problem solving can provide scaffolding for knowledge and skill acquisition and opportunities for meta-cognition. As an example, a beginning student who has learned to reason with equations can invoke Newton's second law in mathematical form *explicitly* to calculate the normal force in terms of the tension and weight and then reason conceptually using this equation to conclude that the tension in the cable is greater than the weight of the elevator accelerating upward. On the other hand, a physics expert can use the same law *implicitly* without using quantitative tools and be confident in conceptually arguing that the upward acceleration implies that tension must exceed the weight. Similarly, a student who does not know whether the maximum safe driving speed while making a turn on a curved horizontal road depends on the mass of the vehicle will have great difficulty reasoning without equations that the maximum speed does not depend on the mass. However, again in this situation, if students are asked to make conceptual inferences after solving a quantitative problem involving maximum safe driving speed, appropriate scaffolding support can help them build a good knowledge structure and develop their reasoning and meta-cognitive skills.

The ICQUIP framework is important for physics instruction at all levels for physics majors (and courses for science and engineering majors in general) because several researchers have conducted investigations which suggest that students often perform well on quantitative problems but not on isomorphic conceptual questions. In a study on student understanding of diffraction and interference concepts, the group that was given a quantitative problem performed significantly better than the group given a similar conceptual question [50]. In another study, Kim et al. examined the relation between traditional physics textbook-style quantitative problem solving and conceptual reasoning [51]. They found that, although students in a mechanics course on average had solved more than 1000 quantitative problems and were facile at mathematical manipulations, they still had many common difficulties when answering conceptual questions on related topics. When Mazur gave a group of Harvard students quantitative problems related to power dissipation in a circuit, students performed significantly better than when an equivalent group was given conceptual questions about the relative brightness of light bulbs in similar circuits [52]. In solving the quantitative problems given by Mazur, students applied Kirchhoff's rules to write down a set of equations and then solved the equations algebraically for the relevant variables from which they calculated the power dissipated. When the conceptual circuit question was given to students in similar classes, many students appeared to guess the answer rather than reason about it systematically. For example, if students are given quantitative problems about the power dissipated in each (identical) headlight of a car with resistance R when the two bulbs are connected in parallel to a battery with an internal resistance r and then asked to repeat the calculation for the case when one of the headlights is burned out, the procedural knowledge of Kirchhoff's rules can help students solve for the power dissipated in each headlight even if they cannot conceptually reason about the current and voltage in different parts of the circuit. To reason without resorting explicitly to mathematical tools (Kirchhoff's rules) that the single headlight in the car will be brighter when the other headlight is burned out, students have to reason in the following manner: The equivalent resistance of the circuit is lower when both headlights are working so that the current coming out of the battery is larger. Hence, more of the battery voltage drops across the internal resistance r and less of the battery voltage drops across each headlight and therefore each headlight will be less bright. If a student deviates from this long chain of conceptual reasoning required, the student may not make a correct inference. Prior research in mechanics [45] also suggests that many students were reluctant to convert a problem posed conceptually into a quantitative problem even when explicitly asked to do so because due to lack of expertise, the task of first converting a conceptual problem to a quantitative problem is cognitively demanding [49] (even though they were more likely to obtain the correct answer by integrating conceptual and quantitative approaches). The students often used their gut feelings rather than explicitly invoking relevant physics concepts or principles for the conceptual problems. On the other hand, appropriate integration of conceptual and quantitative understanding as emphasized in the ICQUIP framework can provide opportunity for metacognition and expertise development.

Prior research suggests that the situation in advanced quantum mechanics courses is similar [53-55]. For example, in surveys administered to 89 advanced undergraduates and more than two hundred graduate students from seven universities enrolled in quantum mechanics courses, students were given a problem in which the wave function of an electron in a one-dimensional infinite square well of width *a*, at time *t* = 0 in terms of stationary states is given by $\Psi(\mathrm{x},0) = \sqrt{\frac{2}{7}}\phi_1 + \sqrt{\frac{5}{7}}\phi_2$ [53-56]. They were asked to write down the possible values of the energy and the probability of measuring each and then calculate the expectation value of energy in the state $\Psi(\mathrm{x},\mathrm{t})$. Although 67% of the students correctly noted that the probability for the outcome of the ground state energy E_1 is $\frac{2}{7}$ and the first excited state energy E_2 is $\frac{5}{7}$, a majority were unable to use this information to determine the expectation value of energy $\frac{1}{7}(2E_1 + 5E_2)$. Not only did the correct responses decrease from 67% to 39%, the students who calculated the expectation value $\langle E \rangle$ correctly mainly exploited brute-force methods: first writing $\langle E \rangle = \int_{-\infty}^{\infty} \langle \Psi | \hat{H} | \Psi \rangle \, dx$, then expressing $\Psi(\mathrm{x}, \mathrm{t})$ in terms of the two energy eigenstates, then acting $\hat{H}$ on the eigenstates, and finally using orthogonality to obtain the final answer. Some got lost early in this process while others did not remember some other mechanical step, e.g., taking the complex conjugate of the wave function, using orthogonality of stationary states or not realizing the proper limits of the integral. Interviews reveal that many students did not know or recall the qualitative interpretation of expectation value as an ensemble average, and did not realize that the expectation value could be calculated more simply in this case by taking advantage of the first part. Other questions posed to advanced students in quantum mechanics confirmed that many of the difficulties students have are conceptual in nature [55]. For example, analogous difficulties were also observed in response to conceptual questions about Larmor spin precession, especially with regard to the expectation values of spin components and their time dependence, given a particular initial state [55,56]. Interestingly, course instructors were often surprised and noted that on similar but exclusively quantitative calculations, student performance was significantly higher. These examples demonstrate that quantitative facility in problem solving does not automatically imply conceptual understanding in quantum mechanics, and students can master complex calculational problems using algorithmic approaches without understanding the underlying quantum physics concepts. In this sense, from the introductory to advanced levels, conceptual understanding, which is critical for physics expertise development, is much more challenging than facility with the technical aspects if students are mathematically savvy. Moreover, it is important to realize that similar to the plug and chug approaches to problem solving in introductory physics, strict quantitative exercises in advanced courses often fail to provide adequate incentive and opportunity for metacognition and drawing meaningful inferences from the problem solving process to repair, organize and extend one's knowledge structure.

The ICQUIP framework focuses on the fact that in order to learn physics and develop reasoning skills with quantitative tools, students must be given adequate opportunity to interpret symbolic equations and draw qualitative inferences from them. Without this explicit focus on integration of conceptual and quantitative aspects of physics learning, quantitative problem solving can become a mere mathematical exercise instead of an opportunity to develop reasoning skills and "compile" new knowledge of physics as the examples to which the preceding paragraphs have alluded. In other words, for problem solving to be effective and useful for developing a good knowledge structure of physics, students must be given incentives and support to utilize effective problem solving strategies and combine conceptual and quantitative understanding. Unfortunately, without explicit guidance and support, many students solve physics problems using superficial clues and cues, and apply concepts essentially by pattern matching. It is important to recognize that many traditional physics courses *reward* the algorithmic problem solving strategies many students utilize. Many instructors implicitly assume that students know that conceptual analysis and decision making or planning, evaluation of the plan, and reflection on the problem solving process are as important as the implementation phase of the quantitative problem solution. Consequently, they do not explicitly emphasize these strategies which involve making appropriate math-physics connection while solving quantitative problems during their lectures nor do they typically assign conceptual problems in quizzes or exams that require students to think as opposed to solve problems using plug and chug approaches. In introductory physics courses for science and engineering majors, recitation time is usually taught by the teaching assistants who present quantitative homework solutions on the blackboard while students copy them in their notebooks. There is no mechanism in place in a traditional physics courses at all levels to ensure that students make a conscious effort to interpret the physical laws and concepts, make conceptual inferences from the quantitative problem solving tasks, relate the new concepts to their prior knowledge and build a robust knowledge structure. The examples in the preceding paragraphs attest to this fact that many students perform well on quantitative problems by memorizing algorithms and procedures without actually understanding the underlying physics concepts. Good performance on quantitative problems using plug and chug approaches not only gives students the false impression that they are learning and acquiring usable knowledge; these types of calculational problems can lull instructors into thinking that their students are developing a functional understanding of physics, even if they are not. In fact, in one research study we found that physics Ph.D. students in a graduate level core course in electricity and magnetism performed only marginally better than introductory physics students on conceptual questions and had similar conceptual difficulties to introductory students [57]. The ICQUIP framework has important instructional implications particularly because many traditionally taught physics courses do not explicitly help students learn effective problem solving strategies and focus on how to help them develop a robust knowledge structure that necessitates appropriate reflection on both the conceptual and quantitative aspects of the physics problems.

One effective approach for developing and implementing curricula that integrate conceptual and quantitative understanding in physics consistent with the ICQUIP framework can implement quantitative problem solving followed by conceptual problem solving based upon a careful analysis of the underlying knowledge inherent in the quantitative problems commensurate with students' prior knowledge and skills. These conceptual problems can force students to make qualitative inferences from the quantitative problems they just solved. Particular attention should be given to designing conceptual questions which probe common misconceptions and challenge students to make discrimination between concepts which can easily be misinterpreted. Protocols can be designed to help students with the reasoning and planning necessary for a class of problems. For example, to draw inferences about electrostatic forces from a given charge configuration, the protocol can have the concepts, physics laws, and the path that links them, e.g., charge → electric field → superposition of electric field → force, where each arrow can show the nature of the relationship between the adjacent concepts. The field-tested cognitive apprenticeship model [58] can be used to help students learn productively from integrated conceptual and quantitative problem solving. The instructor can constantly model the analysis, planning, implementation, evaluation, and reflection phases of problem solving during lectures, and ensure that students engage in effective problem solving strategies through the use of appropriate rewards. The reflection phase of the problem solving can focus on strategies for making conceptual inferences from symbolic equations and on helping students contemplate how those strategies help them extend their current knowledge [6]. Students can be required to solve coupled quantitative and conceptual problems in homework and recitations after instructors' modeling of the approach. "Scaffolding" can be an important component of instruction to ensure that students develop independence while maintaining good discipline. Initially, the instructor can provide guided practice with prompt, appropriate feedback and support, but the frequency and rigor can decrease as students become better at employing the strategies.

Indeed, prior research suggests that one effective instructional strategy consistent with the ICQUIP framework for reducing conceptual difficulties and helping students develop a functional understanding of physics involves using problems that combine quantitative and conceptual problem solving [45]. Here, by conceptual difficulties, we refer to the difficulties in using one's knowledge to interpret, explain and draw inferences while answering qualitative questions in different physics contexts. For example, we performed a controlled study in introductory physics in which we posed only conceptual problems to some students and quantitative/conceptual problem pairs to others [45]. In one conceptual problem, students were asked to compare the momenta (mass times velocity) of two ships of different masses pulled by two identical tugboats in the same fashion. The other group was first given a quantitative problem in which students had to find an algebraic expression for the momentum of a ship with mass m starting from rest and pulled by a tugboat with a constant force F over a distance d in a time t. Among 65 students who were only posed the qualitative problem, only 16% provided the correct response. Among students who were posed both problems, 56% and 52% provided the correct responses to the quantitative and conceptual problems, respectively [45]. The significant improvement in the performance on the conceptual problem and discussions with students suggests that when they were posed both problems, many students recognized their similarity and took advantage of their quantitative solution to solve the conceptual problem. After solving the quantitative problem, many students recognized that the final momenta of the ships were independent of their masses under the given conditions. Then, they were able to use that knowledge to answer the conceptual problem correctly. Similarly, after recognizing that students in his introductory physics courses had not developed a functional understanding, Mazur restructured his course and focused on qualitative reasoning by posing conceptual questions to students during lectures and also emphasized such reasoning on examinations. Student performance on conceptual problems improved significantly [52]. Additionally, if quantitative problems were still included in the homework and recitation and contribute to the course grade, emphasizing conceptual understanding in lectures also improved the performance on quantitative problems (although the increase was not as much as for the conceptual problems). Similar results have been obtained by replacing traditional recitations which emphasize quantitative problem solving with conceptual tutorials [50] for traditionally taught classes that heavily focus on quantitative problem solving. Students perform significantly better on conceptual problems but they also performed at least as well or better on the quantitative problems.

6.1.3 Developing expertise in advanced physics

While learning physics is challenging even at the introductory level because it requires drawing meaningful inferences and unpacking and applying the few fundamental physics principles, which are in compact mathematical forms, to diverse situations [6], learning upper-level physics is also challenging because one must continue to build on all of the prior knowledge acquired at the introductory and intermediate levels. In addition, the mathematical sophistication required is generally significantly higher for upper-level physics. In order to develop a functional understanding, students must focus on the physics concepts while solving problems and be able to go back and forth between the mathematics and the physics, regardless of whether they are converting a physical situation to a mathematical representation or contemplating the physical significance of the result of a complex mathematical procedure during problem solving. Advanced students may possess a large amount of compiled knowledge about introductory physics due to repetition of the basic content in various courses and may not need to do much self-monitoring while solving introductory problems. Therefore, although much remains to be understood about the nature of expertise in advanced physics, the task of evaluating how expertise develops in advanced physics and whether the self-monitoring skills of advanced students is better than introductory physics students should involve physics topics at the periphery of advanced students' understanding.

6.1.4 Developing expertise in quantum mechanics

Research suggests that learning quantum mechanics is especially challenging for advanced students partly due to the abstract and non-intuitive nature of the subject matter. It is difficult to visualize and reason about quantum concepts especially because one does not generally observe quantum phenomena in everyday experience and the formalism of quantum mechanics is unintuitive. Several prior studies have found that many upper-level undergraduate and graduate students struggle with the foundational concepts in quantum mechanics. Pedagogical approaches have focused on helping students learn quantum mechanics better [e.g., see refs. 59-108].

Prior research also demonstrates that the patterns of difficulties in the context of quantum mechanics bear a striking resemblance to those found in introductory classical mechanics [91]. These analogous patterns of difficulties are often due to the diversity in the goals, motivation, and prior preparation of upper-level students (i.e., the fact that even in an upper-level physics course, students may be inadequately prepared, have unclear goals, and may need extrinsic motivation to engage with learning) [109] as well as the "paradigm shift" from classical mechanics to quantum mechanics. Among upper-level courses, quantum mechanics can be especially challenging for students because the paradigms of classical mechanics and quantum mechanics are very different [91]. For example, unlike classical physics, in which position and momentum are deterministic variables, in quantum mechanics they are operators that act on a wave function (or a state) which lies in an abstract Hilbert space. In addition, according to the Copenhagen interpretation, which is most commonly taught in quantum mechanics courses, an electron in a hydrogen atom does not, in general, have a definite distance from the nucleus; it is the act of measurement that collapses the wave function and makes it localized at a certain distance. If the wave function is known right before the measurement, quantum theory only provides the probability of measuring the distance in a narrow range. The significantly different paradigms of classical mechanics and quantum mechanics suggest that even students with a good knowledge of classical mechanics will start as novices and gradually build their knowledge structure about quantum mechanics. The "percolation model" of expertise can be particularly helpful in knowledge-rich domains such as physics [38]. In this model of expertise, a person's long term memory contains different "nodes" which represent different knowledge pieces within a particular knowledge domain. Experts generally have their knowledge hierarchically organized in pyramid-shaped schema in which the top nodes are more foundational than nodes at a lower level and nodes are connected to other nodes through links that signify the relation between those concepts. As a student develops expertise in a domain, links are formed which connect different knowledge nodes. If a student continues her effort to organize, repair, and extend her knowledge structure, she will reach a percolation threshold when all knowledge nodes become connected to each other by at least one link in an appropriate manner. At this point, the student will become at least a nominal expert. The student can continue on her path to expertise with further strengthening of the nodes and building additional appropriate links. Redundancy in appropriate links between different nodes is useful because it provides alternative pathways during problem solving when other pathways cannot be accessed, e.g., due to memory decay. As a student starts to build a knowledge structure about quantum mechanics, her knowledge nodes will not be appropriately connected to other nodes farther away, and her reasoning about quantum mechanics will only be locally consistent and lack global consistency [38]. In fact, a person who begins a pursuit of expertise in any knowledge-rich domain must go through a phase in which her knowledge is in small disconnected pieces which are only locally consistent but lack global consistency, leading to reasoning difficulties. Therefore, introductory students learning classical mechanics and advanced students learning quantum mechanics are likely to show similar patterns of reasoning difficulties as they strive to move up along the expertise spectrum in each of these sub-domains of physics.

6.1.5 Goal, motivation, and theoretical framework for this investigation

The investigation reported here is based on the hypothesis that consistent with the ICQUIP framework, even in the advanced courses such as quantum mechanics, integrating conceptual and quantitative understanding can help students build a more coherent knowledge structure of physics and develop their reasoning and meta-cognitive skills. The goal of the research is to analyze the impact of incorporating mathematical rigor in a Quantum Interactive Learning Tutorial (QuILT), which consists of research-validated inquiry-based learning sequences, on students' conceptual understanding of quantum optics in the context of the Mach Zehnder Interferometer (MZI) with single photons and polarizers [93,95,110]. We developed and validated a QuILT on the MZI with single photons and polarizers that strives to help students learn about foundational issues in quantum mechanics using an integrated conceptual and quantitative approach (called the hybrid QuILT from now on for convenience) for developing functional understanding and compared student performance after engaging with this QuILT with student performance after another research-validated QuILT on the same topic which only uses conceptual inquiry-based learning sequences. The conceptual QuILT developed earlier focuses on engaging students with conceptual reasoning *only* under the assumption that the underlying quantum mechanics concepts involving single-photon interference and quantum eraser are sufficiently complex that incorporating quantitative tools involving product states of path and polarization may cause cognitive overload for students [49]. However, as the ICQUIP framework emphasizes, developing a good knowledge structure of physics without using quantitative tools can be particularly difficult for students who are not experts because equations can actually provide constraints to help students do appropriate sense making. In the hybrid QuILT, research on student difficulties was used as a guide and the QuILT uses a scaffolded inquiry-based approach to learning and asks students to make conceptual inferences from quantitative tools. Since the learning goals of the hybrid QuILT pertaining to conceptual understanding are the same as for the conceptual QuILT [93,95], after traditional instruction in relevant concepts and after the hybrid QuILT, students were administered the same pre-/posttests (see the Appendix) to evaluate their conceptual understanding as those who had engaged with the conceptual QuILT on the same topic in earlier years. In other words, our goal is to investigate the extent to which students who engaged with the hybrid QuILT learned the underlying concepts.

The reason the MZI with single photons was selected as the context for this investigation is that in the past few decades, quantum optics has emerged as a vibrant research area and single photon experiments have played an important role in elucidating the foundational issues in quantum mechanics. The MZI experiments with single photons and polarizers provides students an opportunity to learn the fundamentals of quantum mechanics in a concrete context [e.g., see refs. 93,95,110], e.g., these experiments elegantly illustrate the wave-particle duality of a single photon, single photon interference, and the probabilistic nature of quantum measurement.

We note that the interpretation of these experiments using quantitative tools involves making conceptual inferences using product states of path and polarization, but the underlying concepts can be taught qualitatively using only conceptual reasoning. We also note that both the conceptual and hybrid versions of the MZI QuILT use visualization tools (simulations) involving the MZI with single photons and polarizers to help students learn about single photon interference and quantum spookiness, e.g., spookiness involving a quantum eraser. Both versions of the QuILT focus on using different contexts of the MZI experiment to help students learn topics such as the wave-particle duality of a single photon, interference of a single photon with itself, and the probabilistic nature of quantum measurements. Students also learn how adding photo-detectors and optical elements such as beam-splitters and polarizers in the paths of the MZI affect the measurement outcomes. The difference between the two versions is that in the hybrid version some of the guided learning sequences involving conceptual reasoning only are replaced by those sequecnes involving both conceptual and quantitative reasoning. This is done with the assumption that advanced students in quantum mechanics courses will benefit from the opportunity to make qualitative inferences from quantitative tools and will not have a cognitive overload despite increased mathematical sophistication of the hybrid QuILT because the learning sequences are research-validated and appropriately scaffolded. The findings of this research also have implications for understanding the nature of expertise in advanced quantum mechanics.

The rest of the paper is organized as follows. We first discuss the background material pertaining to the MZI with single photons and polarizers that both versions of the MZI QuILT strive to help students learn. Next we discuss methodology for the development, validation and in-class implementation of the hybrid QuILT, followed by an overview of the QuILT and how it addresses common conceptual difficulties found via research. We compare the data with those obtained earlier for the conceptual only QuILT on the same topic and conclude with a discussion and summary. Our findings suggest that students perform at least as well or better on questions that require conceptual reasoning after engaging with the hybrid MZI QuILT that combines conceptual and quantitative problem solving compared to when they engaged with the conceptual only QuILT on the same topic.

6.2 BACKGROUND ON THE MACH-ZEHNDER INTERFEROMETER WITH SINGLE PHOTONS

This section summarizes the MZI experiments that students learn about in the QuILT as a vehicle for learning foundational quantum mechanics concepts [93,95,110]. Figure 6.2 shows the MZI setup. For simplicity, the following assumptions are made: 1) all optical elements are ideal; 2) the non-polarizing beam-splitters (BS1 and BS2) are infinitesimally thin such that there is no phase shift when a single photon propagates through them; 3) the monochromatic single photons travel the same distance in vacuum in the upper path (U) and lower path (L) of the MZI; and 4) the initial MZI without the phase shifter is set up such that there is completely constructive interference at photo-detector 1 (D1) and completely destructive interference at photo-detector 2 (D2).

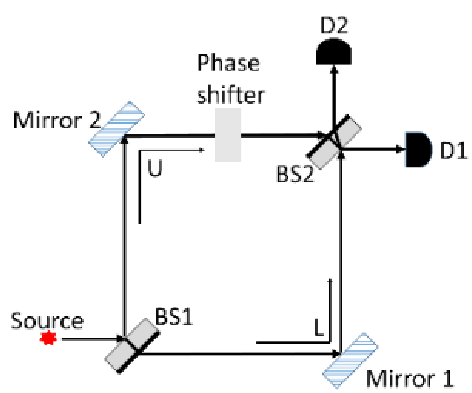


Figure 6.2 MZI setup with a phase shifter in the U path

If single photons are emitted from the source in Figure 6.2, BS1 causes each single photon to be in a superposition state of the path states U and L. The photon path states reflect off the mirrors and recombine at beam-splitter BS2. BS2 mixes the photon path states such that each component of the photon state along the U and L paths can be projected into the photo-detectors D1 and D2 in Figure 6.2. The projection of both components leads to interference at the photo-detectors (called detectors from now on). Depending on the thickness of the phase shifter, interference observed at detectors D1 and D2 can be constructive, destructive, or intermediate. Observing interference of a single photon with itself at D1 and D2 can be interpreted in terms of not having “which-path” information (WPI) about the single photon [93,95,110]. WPI is a common terminology associated with these types of experiments popularized by Wheeler [110]. WPI is unknown (as in the setup shown in Fig. 6.1) if both components of the photon state can be projected into D1 and D2 and the projection of both components at each detector leads to interference. When WPI is unknown and a large number of single photons are sent through the setup, if a phase shifter is inserted in one of the paths of the MZI (as in the U path in Fig. 6.1) and its thickness is varied, the probability of the photons arriving at D1 and D2 will change with the thickness of the phase shifter due to interference of the components of the single photon state from the U and L paths.

In a simplified quantum mechanical model of a photon state which accounts for the two paths U and L (see Fig. 6.2), a single photon traveling through the MZI can be considered to be a two state quantum system. If a basis is chosen in which the state of the photon in the upper state is denoted by $|\mathrm{U}\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and the state of the photon in the lower state is denoted by $|\mathrm{L}\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ (and we arbitrarily denote the initial state of the photon emitted from the source as $|\mathrm{I}\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, the state of the photon propagating towards detector D1 as path state $|\mathrm{D1}\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, and the state of the photon propagating towards detector D2 as the path state $|\mathrm{D2}\rangle = \begin{pmatrix}0\\1\end{pmatrix}$), the matrix representations of the quantum mechanical operators that correspond to beam-splitter 1 [BS1], beam-splitter 2 [BS2], the mirrors [M], and a phase shifter in the upper path $[\mathrm{PS_U}]$ when the basis vectors are chosen in the order $|\mathrm{U}\rangle$, $|\mathrm{L}\rangle$ are: $[\mathrm{BS1}] = \frac{1}{\sqrt{2}}\begin{bmatrix}-1 & 1\\ 1 & 1\end{bmatrix}$, $[\mathrm{BS2}] = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & -1\\ 1 & 1\end{bmatrix}$, $[\mathrm{M}] = \begin{bmatrix}-1 & 0\\ 0 & -1\end{bmatrix}$, and $[\mathrm{PS_U}] = \begin{bmatrix}e^{i\phi_{PS}} & 0\\ 0 & 1\end{bmatrix}$, where ϕ_{PS} is the phase shift introduced by the phase shifter.

In front of BS1 and after BS2, this article and associated QuILT materials use definitions of the U and L paths as follows. The sources shown in figures of this article are all defined as U path, while a source perpendicular to these would be defined as L path. Beyond BS2—or, for cases where it is absent, where BS2 would be—the path directed toward D1 is defined as the U path, while the path directed toward D2 is defined as the L path.

The final state of a photon $|\mathrm{F}\rangle$ in Figure 6.2 can be determined by operating on the initial photon state with the operators corresponding to the optical elements in the appropriate time-ordered manner: $|\mathrm{F}\rangle = [\mathrm{BS2}][\mathrm{PS_U}][\mathrm{M}][\mathrm{BS1}]|\mathrm{I}\rangle = \frac{1}{2}\begin{pmatrix}e^{i\phi_{PS}} + 1\\ e^{i\phi_{PS}} - 1\end{pmatrix}$. The probability of detector D1 registering a photon is $|\langle \mathrm{D1}|\mathrm{F}\rangle|^2 = (1 + \cos\phi_{\mathrm{PS}})/2$ (the probability of detector D2 registering a photon is $|\langle \mathrm{D2}|\mathrm{F}\rangle|^2 = (1 - \cos\phi_{\mathrm{PS}})/2$). Since the probability of a detector registering a photon depends on the phase shift of the phase shifter, interference effects are observed when the phase shift of the phase shifter is gradually changed. If there is no phase shifter in the upper path in Fig. 6.1 ($\phi_{\mathrm{PS}} = 0$), all photons are registered at detector D1 ($|\mathrm{F}\rangle = |\mathrm{D1}\rangle = \begin{pmatrix}1\\0\end{pmatrix}$) since completely constructive interference takes place at detector D1 and completely destructive interference takes place at detector D2.

On the other hand, if the components of the photon path state are not recombined, there is no possibility for interference of the photon path states to occur at the detectors. In this case, WPI is known about a photon that arrives at a detector D1 or D2. In other words, WPI is "known" about a photon if only one component of the photon path state can be projected into each detector. For example, if BS2 is removed from the setup (see Fig. 6.3), WPI is known for all single photons arriving at the detectors because only the component of a photon state along the U path can be projected in D1 and only the component of a photon state along the L path can be projected in D2. When WPI is known, each detector (D1 and D2) has the same probability of clicking. A detector clicks when a photon is detected by it and is absorbed (the state of the single photon collapses, i.e., the single photon state is no longer in a superposition of the U and L path states). However, when WPI is known, there is no way to know a priori which detector will click when a photon is emitted until the photon state collapses either at D1 or at D2 with equal likelihood. When WPI is known, changing the thickness of a phase shifter in one of the paths will not affect the probability of each detector clicking when photons are registered (equal probability for all thicknesses of the phase shifter).

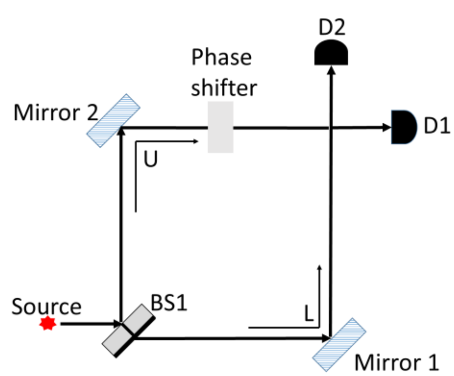


Figure 6.3 MZI setup with beam-splitter 2 (BS2) removed

If beam-splitter 2 is removed (see Fig. 6.3), the final state of the photon is $|\mathrm{F}\rangle = [\mathrm{PS_U}][\mathrm{M}][\mathrm{BS1}]|\mathrm{I}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\phi_{PS}} \\ -1 \end{pmatrix}$. The probability of detector D1 registering a photon is $|\langle \mathrm{D1}|\mathrm{F}\rangle|^2 = 1/2$ (the probability of detector D2 registering a photon is also $1/2$). Thus, the probability of the detectors registering a photon does not depend on the phase shift of the phase shifter and interference effects are not observed when the phase shift of the phase shifter is gradually changed.

When polarizers are added to the MZI setup, they can affect (and even eliminate or reinstate) the interference of a single photon with itself at the detectors [93,95,110]. In all the MZI setups discussed, it is assumed that the detectors are polarization sensitive and the single photons are linearly polarized. In Figure 6.4, two orthogonal polarizers are placed in the U and L paths of the MZI. If the source emits a large number (N) of +45° polarized single photons, $\mathrm{N}/2$ photons are absorbed by the polarizers. If a detector in Fig. 6.4 measures a vertically polarized photon, only one component of the photon path state can be projected in the detector (i.e., the L path state) and WPI is known. If a detector measures a horizontally polarized photon, again, only one component of the photon path state can be projected into the detector (i.e., the U path state) and WPI is known. WPI is known for all photons arriving at the detectors, and there is an equal probability of each detector registering a photon ($\mathrm{N}/4$ photons arrive at each detector). There is no interference observed at the detectors. Inserting a phase shifter and changing its thickness gradually will not affect the number of photons arriving at the detectors in Fig. 6.4.

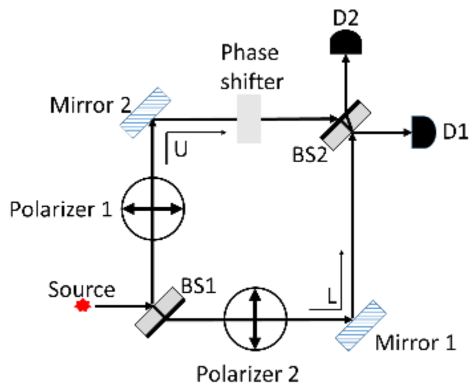


Figure 6.4 MZI setup with a polarizer with a horizontal transmission axis placed in the U path and a polarizer with a vertical transmission axis placed in the L path

If we only consider photon polarization states, the polarization state of a vertically polarized photon can be denoted by $|\mathrm{V}\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and the polarization state of a horizontally polarized photon can be denoted by $|\mathrm{H}\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. These two polarizations are linearly independent and all other photon polarizations can be constructed from these states, e.g., $|+45°\rangle = (|\mathrm{V}\rangle + |\mathrm{H}\rangle)/\sqrt{2}$. The Hilbert space involving both path states and polarization states is a product space. The product space of the polarization states $|\mathrm{V}\rangle$ and $|\mathrm{H}\rangle$ and the path states $|\mathrm{U}\rangle$ and $|\mathrm{L}\rangle$ is four dimensional, and the basis vectors are $|\mathrm{U}\rangle \otimes |\mathrm{V}\rangle = |\mathrm{UV}\rangle$, $|\mathrm{U}\rangle \otimes |\mathrm{H}\rangle = |\mathrm{UH}\rangle$, $|\mathrm{L}\rangle \otimes |\mathrm{V}\rangle = |\mathrm{LV}\rangle$, $|\mathrm{L}\rangle \otimes |\mathrm{H}\rangle = |\mathrm{LH}\rangle$. If the initial path state of the photon emitted from the source is denoted by $|\mathrm{I}\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and the initial polarization state of the photon is $|+45°\rangle = (|\mathrm{V}\rangle + |\mathrm{H}\rangle)/\sqrt{2}$, in the 4×4 product space, the initial state of the photon $|\mathrm{I}_{45°}\rangle$ is $|\mathrm{I}_{45°}\rangle = |\mathrm{I}\rangle \otimes |45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix}$. The matrix representations of the quantum mechanical operators that correspond to beam-splitter 1 [BS1], beam-splitter 2 [BS2], the mirrors [M], a phase shifter in the upper path [$\mathrm{PS_U}$], a horizontal polarizer in the upper path [$\mathrm{P_{UH}}$], a vertical polarizer in the lower path $[P_{LV}]$, and a +45 polarizer in the path between BS2 and detector D1 $\left[P_{D1,+45^\circ}\right]$ when the basis vectors are chosen in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$ are:

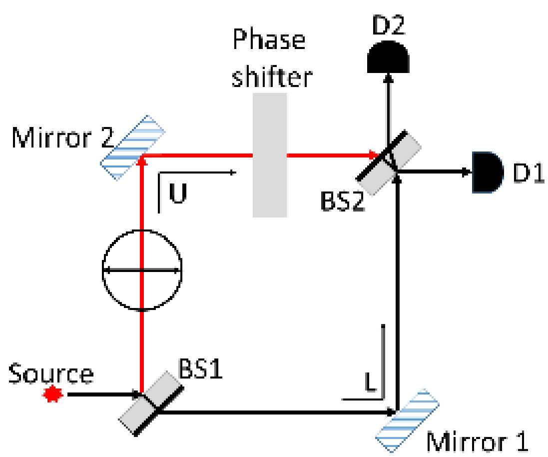
$$[BS1] = \frac{1}{\sqrt{2}}\begin{bmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix},\ [BS2] = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix},\quad [M] = -\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = -\hat{I},$$

$[PS_U] = \begin{bmatrix} e^{i\varphi_{ps}} & 0 & 0 & 0 \\ 0 & e^{i\varphi_{ps}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$, where ϕ_{PS} is the phase shift introduced by the phase shifter,

$[P_{UH}] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$, and $[P_{LV}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$.

Thus, the final state of a photon $|F\rangle$ in Figure 6.4 can be determined by operating on the initial photon state with the operators corresponding to the optical elements in the appropriate time-ordered manner: $|F\rangle = [BS2][PS_U][M][P_{LV}][P_{UH}][BS1]|I_{45^\circ}\rangle = (|UV\rangle + e^{i\varphi_{PS}}|UH\rangle - |LV\rangle + e^{i\varphi_{PS}}|LH\rangle)/(2\sqrt{2})$. The probability of detector D1 registering a horizontally polarized photon is $\left|e^{i\varphi_{PS}}/(2\sqrt{2})\right|^2 = 1/8$ and the probability of detector D1 registering a vertically polarized photon is $\left|-1/(2\sqrt{2})\right|^2 = 1/8$. The total probability of detector D1 registering a photon is $1/8 + 1/8 = 1/4$. The total probability of detector D2 registering a photon is also $1/4$. Thus, in the case shown in Figure 6.4, the probability of a detector registering a horizontally or vertically polarized photon does not depend on the phase shift of the phase shifter and interference effects are not observed when the phase shift of the phase shifter is gradually changed.

In Figure 6.5, only one polarizer is present. Unlike the situation in Figure 6.4, which-path information is not known for all photons in the situation in Figure 6.5. Here, the final state of the photon after it propagates through the beam splitter BS2, but before it reaches the detectors is: $\frac{1}{2\sqrt{2}}\big(|U\rangle|V\rangle + \big(e^{i\varphi_{PS}} + 1\big)|U\rangle|H\rangle - |L\rangle|V\rangle + (e^{i\varphi_{PS}} - 1)|L\rangle|H\rangle\big)$. If detector D1 is covered by a vertical polarizer, the probability that detector D1 registers a vertically polarized photon is $\frac{1}{8}$ (which-path information is known about these photons arriving at detector D1 and they do not display interference). If the detector D1 is covered by a horizontal polarizer, the probability that detector D1 registers a horizontally polarized photon is $\frac{1+\cos\varphi_{ps}}{4}$ (WPI is unknown about these photons arriving at detector D1 and they display interference). The total probability that detector D1 clicks (if not covered by a polarizer) is $\frac{1}{8} + \frac{1+\cos\varphi_{ps}}{4}$. Also, if detector D2 is covered by a vertical polarizer, the probability that detector D2 registers a vertically polarized photon is $\frac{1}{8}$ (which-path information is known about these photons arriving at detector D2 and they do not display interference). If the detector D2 is covered by a horizontal polarizer, the probability that detector D2 registers a horizontally polarized photon is $\frac{1-\cos\varphi_{ps}}{4}$ (WPI is unknown about these photons arriving at detector D2 and they display interference). The total probability that detector D2 clicks (if not covered by a polarizer) is $\frac{1}{8} + \frac{1-\cos\varphi_{ps}}{4}$.



8 6

Figure 6.5 MZI setup with a polarizer with a horizontal transmission axis placed in the U path

Figure 6.6 shows a quantum eraser setup in which two orthogonal polarizers are placed in the two paths of the MZI and a third polarizer is placed between BS2 and detector D1. The third polarizer has a transmission axis which is different from the two orthogonal polarizers. Without polarizer 3, WPI is known for all photons arriving at the detectors (as in Figure 6.4) and interference is not observed at the detectors. However, when polarizer 3 is inserted between BS2 and detector D1, both the U and L path states are projected into D1 and WPI is unknown for all photons. For example, if detector D1 measures vertically polarized photons (using another polarizer right in front of D1), both components of the photon path state are projected into detector D1 and WPI is unknown. Similarly, if D1 measures horizontally polarized photons, both components of the photon path state are projected into detector D1 and WPI is again unknown. Interference is observed at detector D1. If a phase shifter is inserted into one of the paths of the MZI, changing its thickness gradually will change the number of photons arriving at D1. Because polarizer 3 eliminates WPI at the detector D1, this MZI setup is called a quantum eraser. However, in Fig. 6.6, WPI is known at detector D2 and no interference is observed there. Inserting a phase shifter into one of the paths of the MZI and changing its thickness gradually will not affect the number of photons that arrive at D2.

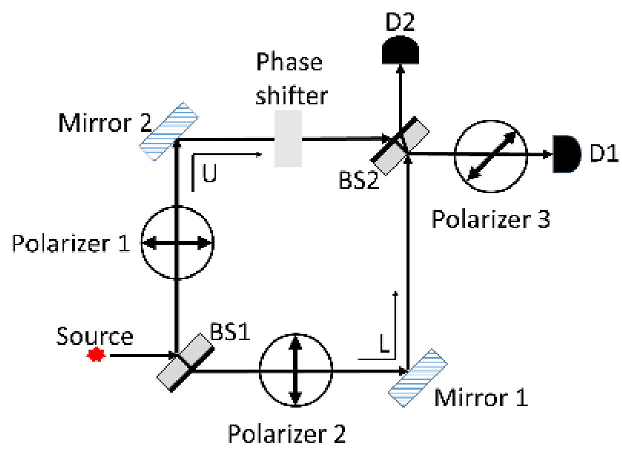


Figure 6.6 Quantum eraser setup

The matrix representing a third polarizer with a +45° polarization axis inserted between beam-splitter 2 and detector D1, $[P_{D1,+45°}]$ (as shown in Figure 6.6) is $[P_{D1,+45°}] = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$. The final state of the photon in Figure 6.6 can be determined by operating on the initial photon state with the operators corresponding to optical elements in the appropriate time-ordered manner:

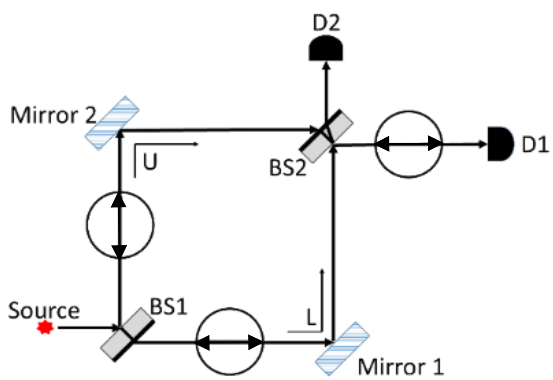
$|F\rangle = [P_{D1,+45°}][BS2][PS_U][M][P_{LV}][P_{UH}][BS1]|I_{45°}\rangle =$

$\left(\left(\frac{1}{2} + \frac{1}{2}e^{i\varphi_{PS}}\right)|UV\rangle + \left(\frac{1}{2} + \frac{1}{2}e^{i\varphi_{PS}}\right)|UH\rangle - |LV\rangle + e^{i\varphi_{PS}}|LH\rangle\right)/(2\sqrt{2}).$

The probability of detector D1 registering a horizontally polarized photon is $\left|(\frac{1}{2} + \frac{1}{2}e^{i\varphi_{PS}})/(2\sqrt{2})\right|^2 = (1 + \cos\varphi_{PS})/16$ and the probability of detector D1 registering a vertically polarized photon is $\left|(\frac{1}{2} + \frac{1}{2}e^{i\varphi_{PS}})/(2\sqrt{2})\right|^2 = (1 + \cos\varphi_{PS})/16$ (the total probability of detector D1 registering a photon is $(1 + \cos\varphi_{PS})/8$).In the quantum eraser case shown in Figure 6.6, the probability of detector D1 registering a horizontally or vertically polarized photon depends on the phase shift of the phase shifter and interference effects are observed when the phase shift of the phase shifter is gradually changed. WPI is unknown at detector D1.

The quantum eraser setup also distinguishes between a stream of unpolarized photons and photons which have been polarized at +45°. If the source emits unpolarized photons, one can consider half of the photons emitted to be vertically polarized and half of the photons emitted to be horizontally polarized (or half of the photons emitted can be considered +45° polarized and half of the photons -45°polarized). In Fig. 6.6, if one considers unpolarized photons as a mixture of half vertically polarized and half horizontally polarized photons incident at BS1 randomly, a single photon with horizontal polarization can only go through the upper path and a single photon with a vertical polarization can only go through the lower path. If the photon passes through polarizer 3, the detector can only project one component of the photon path state and WPI is known. Interference effects are not observed. Inserting a phase shifter and changing its thickness gradually will not affect the number of photons arriving at the detectors. On the other hand, in Fig. 6.7, if one considers unpolarized photons as a mixture of half of the photons polarized at +45° and half of the photons polarized at -45° incident at BS1 randomly, the total probability of unpolarized photons arriving at detector D1 can be determined by averaging the total probabilities of detector D1 registering a photon for the two cases in which the source emits +45° single photons and -45° single photons. In the case in which the source emits +45° single photons, the total probability of detector D1 registering a photon is $(1 + \cos \varphi_{\mathrm{PS}})/8$, as shown earlier. In the case in which the source emits -45° single photons, the total probability of detector D1 registering a photon is $(1 - \cos \varphi_{\mathrm{PS}})/8$. The average of these two probabilities ($(1 + \cos \varphi_{\mathrm{PS}})/8$ and $(1 - \cos \varphi_{\mathrm{PS}})/8$) is $1/8$, indicating that for unpolarized light (which can be treated as a mixture in which half of the photons are +45° polarized and half of the photons are -45° polarized) the setup in Fig. 6.5

does not erase which-path information and changing the phase shift of the phase shifter does not affect the number of photons arriving at the detector D1. However, in the quantum eraser setup (see Fig. 6.6), if the source emits a stream of +45° polarized single photons, both components of the photon path state can be projected in detector D1. The total probability of detector D1 registering a photon is $(1+\cos\varphi_{PS})/8$ and depends on the phase shift of the phase shifter. Interference effects are observed at detector D1. Thus, the quantum eraser distinguishes between a stream of unpolarized photons and photons which have been polarized at +45°. In the quantum eraser setup, interference effects will not be observed at detector D1 when unpolarized photons are emitted and interference effects are observed at detector D1 when polarized photons are emitted.



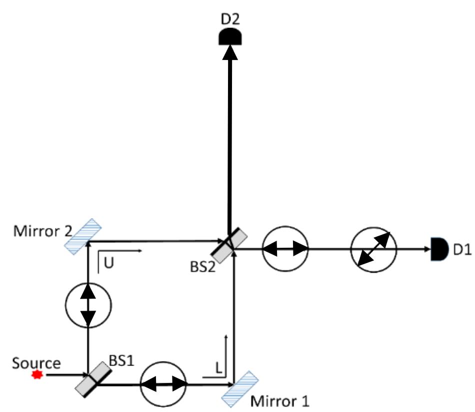


Figure 6.7 The MZI arrangement similar to the quantum eraser setup, but with a horizontal polarizer in place of the 45° polarizer between BS2 and D1 (left) and an additional horizontal polarizer in addition to the 45° polarizer between BS2 and D1 as shown (right)

Figure 6.7 shows two arrangements that share a surface feature with the quantum eraser shown in Figure 6.6. However, photons propagating through either of these arrangements do not display interference in the way that the quantum eraser does because of WPI for all photons. We note that in both versions of the QuILT, students engaged with a situation similar to that in Figure

6.7 on the left-hand side (but with a vertical polarizer right before detector D1). However, the situation in the right hand side of Figure 6.7, which was posed as a question on the pre/posttests, was novel for students in that they had not encountered this situation in traditional instruction or in the QuILT. We wanted to use this context to investigate transfer of learning from the situations students had learned to a new situation [12,45].

6.3 METHODOLOGY FOR DEVELOPMENT AND VALIDATION AND OVERVIEW OF THE QuILT

6.3.1 Methodology for development and validation of the hybrid QuILT

Students who participated in this research were upper-level undergraduates and graduate students in respective core quantum mechanics courses at a large research university. We note that the conceptual QuILT and the corresponding pre/posttests were developed and validated previously [93,95] based upon research on student common difficulties with quantum mechanics concepts in the context of the MZI experiment after instruction in relevant concepts. The hybrid QuILT on the MZI with single photons is inspired by the ICQUIP framework and strives to help students develop a coherent understanding of these concepts in the context of the MZI experiments by integrating conceptual and quantitative understanding explicitly using a guided inquiry-based approach to learning. Similar to the conceptual QuILT, the guided learning sequences in the hybrid QuILT take advantage of the synergistic models that emphasize providing appropriate scaffolding, e.g., the Piagetian model of "optimal mismatch" [111-112], the preparation for future learning or "PFL" framework of Schwartz, Bransford, and Sears [113], and Vygotsky's zone of proximal development or “ZPD” [114]. These models provide guidelines for how to structure the guided learning sequences based upon research on students’ difficulties as well as knowledge of what students are able to do after traditional instruction. Furthermore, a cognitive task analysis of the underlying concepts from an expert perspective [6] was also used as a guide to develop the hybrid QuILT. The cognitive task analysis from an expert perspective involves a careful analysis of the underlying concepts in the order in which those concepts should be invoked and applied in each situation to accomplish a task. The hybrid QuILT actively engages students in the learning process using an inquiry-based approach in which quantitative and conceptual aspects of learning are integrated and various concepts build on each other. The hybrid QuILT can be used in upper-level quantum mechanics courses after students have had instruction in the relevant topics. Here we will focus on its effectiveness for both upper-level undergraduate and graduate quantum mechanics students compared to the conceptual only QuILT on the same topic.

Similar to the conceptual only QuILT, the development of the hybrid QuILT went through a cyclic, iterative process of development and validation which included the following stages before the in-class implementation:

(1) Development of the preliminary version based on a cognitive task analysis of the underlying knowledge and research on student difficulties,

(2) Implementation and evaluation of the QuILT by administering it individually to students and obtaining feedback from faculty members who are experts in these topics,

(3) Determining its impact on student learning and assessing what difficulties were not adequately addressed by the QuILT,

(4) Refinements and modifications based on the feedback from the implementation and evaluation.

In addition to written free-response questions administered to students in various classes, individual interviews with 15 students were carried out using a think-aloud protocol [115] to better understand the rationale for their responses throughout the development of various versions of the hybrid QuILT. Students are asked to predict what should happen in a particular situation. After their predictions, students follow an integrated conceptual and quantitative guided inquiry-based approach to learning. They use a computer simulation to check their predictions and reconcile the differences between those predictions and what the simulation shows. After each individual interview utilizing a particular version of the hybrid QuILT, modifications were made based upon the feedback obtained from the interviewed students. For example, if students got stuck at a particular point and could not make progress from one question to the next with the scaffolding already provided or could not make meaningful conceptual inferences from quantitative tools despite the scaffolding support, suitable modifications were made. Thus, the administration of the hybrid QuILT to the graduate students and upper-level undergraduate students individually was useful to ensure that the guided approach using integrated conceptual and quantitative tools was effective and the questions were unambiguously interpreted. The hybrid QuILT was also iterated with three faculty members several times to ensure that the content and wording of the questions were appropriate. Modifications were made based upon their feedback. When we found that the QuILT was working well in individual administration and the posttest performance was significantly improved compared to the pretest performance, it was administered in upper-level undergraduate and graduate core quantum mechanics classes. The QuILT is best used in class to give students an opportunity to work together in small groups and discuss their thoughts with peers, which provides peer learning support. However, students can be asked to work on the parts they could not finish in class at home as homework or even the entire QuILT as homework.

6.3.2 Overview of the hybrid QuILT

The QuILT begins with a warm-up that builds on students' prior knowledge about the interference of light and then helps students learn about the MZI with single photons using an integrated conceptual and quantitative approach requiring only 2 by 2 matrix mechanics with the upper and lower path states. Then, students transition to the main section of the QuILT that focuses on the fundamentals of quantum mechanics in the context of the MZI with single photons and polarizers using an integrated conceptual and quantitative approach requiring conceptual interpretations of the product states of path and polarization. Students are provided scaffolding as they construct matrices that describe different elements of the MZI. Students then use these matrices to describe various arrangements and to do sense-making of the underlying concepts. Using an integrated conceptual and quantitative approach, the QuILT strives to provide "optimal mismatch" [111] by explicitly bringing out common difficulties found via research [93] and then providing appropriate scaffolding to help students develop a coherent understanding. Throughout the QuILT, students make predictions about a particular MZI setup, work through integrated conceptual and quantitative learning sequences, check their predictions via a computer simulation and reconcile the differences between their predictions and observations. If the students' predictions and observations are inconsistent, further scaffolding is provided throughout the QuILT to ensure that students remain in the "optimal adaptability corridor" [113] or ZPD [114]. Throughout the QuILT, students are given opportunities to reflect on the concepts learned so far in the guided integrated conceptual and quantitative approach to learning and ensure that they are answering the questions correctly.

As an example, despite traditional instruction, students often struggled with the concept of WPI and the relationship between interference of a single photon at the photo-detectors and whether WPI is known or unknown. Therefore, the QuILT gives students an opportunity to use an integrated conceptual and quantitative approach to reason about how WPI about the photons arriving at the detectors D1 and D2 may be known in some situations. Interviews suggest that many students had difficulty with how the interference at D1 and D2 in Fig. 6.2 is affected by placing a single polarizer, e.g., with a vertical polarization axis, in the L path of the MZI. In particular, students had difficulty with the fact that in this situation, if the source emits a large number of unpolarized single photons, there are three possible measurement outcomes at the detectors due to the polarizer: 1) the photon is absorbed by the polarizer and it does not reach the detectors D1 or D2 (25% probability); 2) the photon is not absorbed by the vertical polarizer but both the photon path state and polarization state collapse, i.e., the photon has a 25% probability of being in the U path with a horizontal polarization; and 3) the photon is not absorbed by the vertical polarizer and the polarization state of the photon collapses but not the path state, i.e., the photon has a 50% probability of having a vertical polarization and remaining in a superposition of the U and L path states. If a detector registers a photon with a horizontal polarization, WPI is known since the vertical polarizer collapsed the photon with a horizontal polarization to the U path state. However, WPI is unknown if a detector registers a photon with vertical polarization since the vertical polarizer does not collapse the path state of such a photon and this photon displays constructive interference at D1 and destructive interference at D2 in the given setup without the phase shifter. Thus, D1 will register all single photons with a vertical polarization (50% of photons emitted from the source) and 12.5% of the single photons emitted from the source which collapsed to the horizontal polarization state due to the vertical polarizer in the L path. D2 will register only photons with a horizontal polarization (12.5% of the photons emitted from the source).

The QuILT incorporates these types of difficulties as resources. Student learning is scaffolded via integrating conceptual and quantitative understanding, incorporating quantitative aspects of MZI experiments via 2 by 2 (for path states only when polarizers are absent) or 4 by 4 matrix mechanics (when both path and polarization are present), and reasoning about what will happen at the detectors D1 and D2 for the photon state after passing BS2 (or when BS2 is not there) in different situations. For example, for the situation shown in Fig. 6.4, before being asked about the probability of detectors D1 and D2 clicking when the detectors are not covered by a polarizer (e.g., $|\langle U|\Psi\rangle|^2$) vs. when it is covered by a horizontal or vertical polarizer (e.g., $|\langle UV|\Psi\rangle|^2$ or $|\langle UH|\Psi\rangle|^2$), students are asked to first write the photon state $|\Psi\rangle = \frac{1}{2\sqrt{2}}\begin{pmatrix} 1 \\ e^{i\varphi_{PS}} \\ -1 \\ e^{i\varphi_{PS}} \end{pmatrix}$ right after the photon exits BS2 in terms of the basis vectors chosen, i.e., $\frac{1}{2\sqrt{2}}\left(|U\rangle|V\rangle + e^{i\varphi_{PS}}|U\rangle|H\rangle - |L\rangle|V\rangle + e^{i\varphi_{PS}}|L\rangle|H\rangle\right)$. Then students are guided to connect WPI and whether interference is observed in a given situation to whether the probability of a detector clicking depends on the phase shift introduced by the phase shifter (in this case, none of the probabilities will depend on the phase shift since WPI is known for all photons arriving at the detectors in Fig. 6.3). On the other hand, for the situation in Fig. 6.5, students learn to reason that the photon state after BS2 is given by $\frac{1}{2\sqrt{2}}\left(|U\rangle|V\rangle + \left(e^{i\varphi_{PS}} + 1\right)|U\rangle|H\rangle - |L\rangle|V\rangle + (e^{i\varphi_{PS}} - 1)|L\rangle|H\rangle\right)$ and WPI is known for some of the photons that arrive at D1 and D2 but not for other photons arriving there so some photons display interference while others do not. The QuILT also strives to use the coupled conceptual and quantitative approach to help students reason about the quantum eraser.

Since students struggled with the concepts of whether interference is observed at detectors D1 and D2 in different experimental situations involving the MZI and the collapse of the state of the photon upon measurement, the inquiry-based approach employed in the QuILT strives to scaffold their learning pertaining to these issues. For example, after traditional instruction, many students had difficulties with the fact that, within the MZI, the U and L components of the photon state can interfere at the detectors D1 and D2. To check if interference occurs at the detectors for the MZI setup shown in Figure 6.2, after working through the integrated conceptual and quantitative learning sequences, students are asked to use a computer simulation and reconcile the difference between their predictions and observations. In the computer simulation, a screen is used in place of point detector D1 and the photon has a transverse Gaussian width as opposed to being a collimated beam having an infinitesimally small transverse width. The advantage of the screen (as opposed to point detectors D1 and D2) is that an interference pattern is observed without placing a phase shifter in one of the paths and changing the path length difference between the two paths. For the case with point detectors D1 and D2, the thickness of the phase shifter must be changed in order to observe interference if interference is displayed in a particular experimental situation. Students can use the computer simulation to verify that single photons can exhibit wave properties while propagating through the MZI setup and that the U and L components of the photon state can interfere so that interference fringes are observed on the screen in suitable situations (see Fig. 6.8) as they reasoned using the integrated conceptual and quantitative approach.

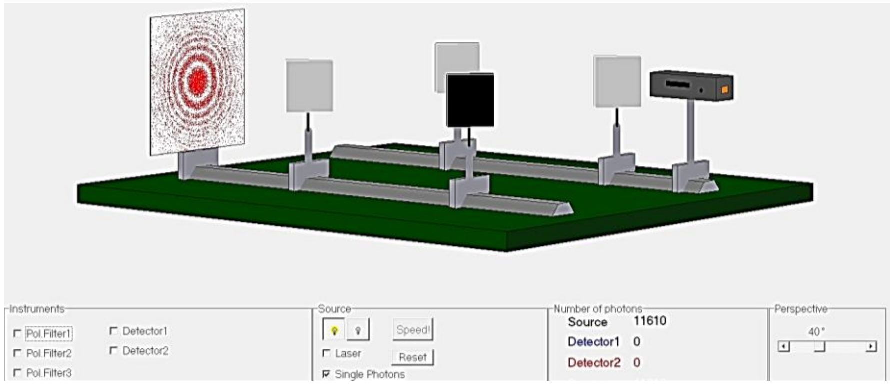


Figure 6.8 Screen shot of the computer simulation of a large number of single photons propagating through the MZI. Simulation developed by Albert Huber.

After working through the integrated conceptual and quantitative QuILT, students are expected to be able to qualitatively reason about how a single photon can exhibit interference. They are also expected to be able to describe how a photon can be delocalized or localized depending on the situation and that the measurement of a photon's position at the detector collapses the photon path state. Students are also expected to be able to explain the roles of BS1, BS2, and additional polarizers placed in the MZI and how these affect the interference at the detectors D1 and D2. Students should also be able to reason about whether a particular MZI setup gives WPI about a single photon and destroys the interference observed at the detectors and whether inserting a phase shifter will change the number of photons arriving at detectors D1 and D2.

6.4 METHODOLOGY FOR IN-CLASS IMPLEMENTATION OF VALIDATED QuILT

The hybrid QuILT about the MZI with single photons includes a pretest to be administered immediately after traditional instruction on the concepts involved in the MZI experiments with single photons and polarizers but before students engage with the QuILT and a posttest is administered after students finish working on the QuILT. The questions on the pretest and posttest, which are identical, are open-ended and were validated earlier [93]. These are provided in the Appendix. The open-ended format requires that students generate answers based upon a robust understanding of the concepts as opposed to memorization of concepts. The same rubric that was used in Ref. [93] for the conceptual QuILT was also used for to grade the work of students who used on the hybrid QuILT. The hybrid QuILT includes the same MZI experiments as the conceptual QuILT [93] except that a situation similar to that shown (see pre/posttest question (4) in the Appendix) with a detector in the U path was not in the hybrid QuILT, but there was an isomorphic situation that students engaged with in the conceptual QuILT with a detector in the L path [93].

Once we determined that the hybrid QuILT was effective in individual administration, it was administered to upper-level undergraduates (mainly physics juniors and seniors) and first year physics graduate students in core quantum mechanics courses at a large research university. Students in two upper-level undergraduate quantum mechanics courses (two consecutive years) and one first year graduate core quantum mechanics course first had traditional lecture-based instruction in relevant concepts. The instructors for all of these courses were different. The instruction by the course instructors included an overview of the MZI setup and students learned about the propagation of light through the beam-splitters, phase difference introduced by the two paths of the MZI, the meaning of what happens when the detectors "click," and the effect of polarizers in various locations of the MZI in different experiments students engage with in the QuILT. We note that similar to Ref. [93], physics education researchers who developed and validated the QuILT did not dictate how the topic of the MZI was to be covered in traditional lecture prior to the administration of the pretest and subsequent engagement with the QuILT.

Instructors were advised on what should be covered before the pretest and provided a suggested grade incentive for student participation on the pretest, QuILT and posttest. Then, students were given the pretest in class. The QuILT warm-up was given as homework. Students worked through part of the hybrid quantitative-qualitative QuILT in class and were given one week to work through the rest of the QuILT as homework. The part of the QuILT that students worked on in class was facilitated for all of the courses by one of the authors of this article who filled in as a guest instructor (she was also the in-class conceptual MZI QuILT facilitator for all of the classes in Ref. [93]). Thus, there was a level of uniformity in the in-class implementation in all of the classes. For both undergraduates and graduate students, the pretest and QuILT counted as a small portion of their homework grade for the course. All students were then administered the posttest in their respective quantum mechanics classes. All students had sufficient time to take the pre-/posttests. The posttests were graded for correctness as a quiz for both the undergraduate and graduate quantum mechanics courses. We note that two graders graded all of the pre/posttests on the rubric and the inter-rater reliability was better than 95%.

We compare the data from the hybrid MZI QuILT with data from the conceptual MZI QuILT from Ref. [93]. We note that the data from undergraduates in Ref. [93] are for the conceptual MZI QuILT implemented in the same upper-level quantum mechanics course for physics juniors and seniors in preceding years. The data from graduate students in Ref. [93] are for first year graduate students who were simultaneously enrolled in the graduate core quantum mechanics course and a semester-long teaching of physics course which is a mandatory pass/fail course, but the pretest, conceptual QuILT and posttest were part of the teaching of physics course to help graduate students learn about the tutorial approach to learning and teaching (since the core graduate quantum mechanics instructor was reluctant to administer these in the graduate quantum mechanics course due to time-constraints). Thus, although the conceptual MZI QuILT was administered in a similar manner to the hybrid MZI QuILT to a similar graduate student population in different years at the same university (first semester physics graduate students), since the conceptual QuILT was administered in a pass/fail course, pre-/posttests and the conceptual MZI QuILT were graded for completeness [93]. We note that the data that were previously reported in Ref. [93] are for two consecutive years of the course for some of the test items, although we compare student performance after engaging with the hybrid MZI QuILT also with data for some test items after the conceptual MZI QuILT that are unpublished.

Table 6.1 Percentages of undergraduates and graduate students who correctly answered questions on the MZI pre/posttest before and after using the hybrid QuILT. Normalized gains and effect sizes (Cohen's d) are shown for each class for each question. Graduate students are matched, while undergraduates had only small fluctuations in participation.

	Graduate Students				Undergraduates Group A				Undergraduates Group B			
Q	Pre(%) N=10	Post(%) N=10	<g>	d	Pre(%) N=24	Post(%) N=20	<g>	d	Pre(%) N=15	Post(%) N=16	<g>	d
1	55	100	1.00	0.67	17	93	0.91	1.21	48	91	0.81	0.54
2	55	82	0.60	0.40	69	89	0.64	0.40	57	84	0.64	0.46
3a	60	95	0.89	0.49	34	100	1.00	1.18	55	100	1.00	0.74
3b	--	--	--	--	--	--	--	--	57	94	0.86	0.53
4a	10	82	0.80	2.33	44	60	0.29	0.34	77	100	1.00	0.92
4b	20	90	0.88	1.98	29	56	0.36	0.54	73	100	1.00	0.85
4c	30	82	0.74	1.22	13	56	0.49	1.01	40	94	0.90	1.39
6	64	80	0.45	0.37	56	75	0.43	0.49	73	97	0.88	0.73
7a	5	68	0.67	3.21	10	60	0.55	1.97	23	47	0.31	0.69
7b	36	85	0.76	1.19	48	95	0.90	1.29	80	81	0.06	0.03
7c	36	73	0.57	0.83	23	65	0.55	1.20	40	59	0.32	0.50
8a	5	95	0.95	6.32	40	83	0.71	1.09	77	91	0.60	0.44
8b	18	90	0.88	2.07	13	40	0.31	0.66	40	88	0.79	1.13
8c	41	91	0.85	1.29	13	35	0.26	0.55	20	81	0.77	1.55
9a	23	91	0.88	2.21	17	65	0.58	1.53	47	88	0.77	1.44
9b	18	90	0.88	2.07	4	80	0.79	2.40	53	97	0.93	1.20
9c	9	82	0.80	2.13	2	58	0.57	1.79	23	88	0.84	1.99
10a	18	91	0.89	2.39	15	68	0.62	1.59	40	94	0.90	1.86
10b	27	90	0.86	1.65	8	45	0.40	0.91	30	88	0.82	1.48
10c	27	91	0.88	1.70	4	50	0.48	1.20	27	84	0.79	1.46
11a	14	91	0.89	2.59	15	45	0.36	0.77	30	84	0.78	1.66
11b	27	90	0.86	1.65	4	35	0.32	0.84	33	75	0.63	0.92
11c	27	82	0.75	1.31	4	35	0.32	0.84	33	69	0.53	0.76
12	18	73	0.67	1.31	4	70	0.69	2.08	36	94	0.90	1.54
Average	33	87	0.80	3.46	27	70	0.60	2.61	48	88	0.77	2.46

Table 6.2 Percentages of undergraduates and graduate students who correctly answered questions on the MZI pre/posttest before and after using the hybrid QuILT after averaging over the sub-parts of each question. Normalized gains are shown for each class for each question.

	Graduate Students			Undergraduates Group A			Undergraduates Group B		
Q	Pre(%) N=25	Post(%) N=10	<g>	Pre(%) N=24	Post(%) N=20	<g>	Pre(%) N=15	Post(%) N=16	<g>
1	55	100	1.00	17	93	0.91	48	91	0.81
2	55	82	0.60	69	89	0.64	57	84	0.64
3	60	95	0.89	34	100	1.00	56	97	0.93
4	20	85	0.81	29	57	0.39	63	98	0.95
6	64	80	0.44	56	75	0.43	73	97	0.88
7	26	75	0.66	27	73	0.63	48	62	0.27
8	21	92	0.90	22	53	0.39	46	87	0.75
9	17	88	0.86	8	68	0.65	41	91	0.85
10	24	91	0.88	9	54	0.50	32	89	0.83
11	23	88	0.84	8	38	0.42	32	76	0.64
12	18	73	0.67	4	70	0.69	36	94	0.90
Average	33	87	0.80	27	70	0.60	48	88	0.77

Table 6.3 Percentages of undergraduates and graduate students who correctly answered questions on the MZI pre/posttest before and after using the conceptual only QuILT after averaging over the sub-parts of each question. Normalized gains are shown for each class for each question (effect sizes were not calculated). Data were primarily taken from Ref. [93], with sub-questions averaged for comparison (we note that a few question numberings differed from the prior study but have been matched appropriately). Unless otherwise specified, the number of graduate students was 45 (matched), the numbers of undergraduates were 44 (pre) and 38 (post), with data collected over a period of two years in both cases. Data marked with an asterisk (*) are previously unpublished data, with 28 graduate students (matched) and 26 undergraduates in pretest and 25 in posttest. Normalized gain is shown for each class.

	Graduate Students			Undergraduates		
Q	Pre(%)	Post(%)	<g>	Pre(%)	Post(%)	<g>
1	21	66	0.57	8	72	0.70
2	41	76	0.59	31	86	0.80
3	18	79	0.74	15	79	0.75
4	50	87	0.74	61	97	0.92
6*	7	59	0.56	31	73	0.61
7*	23	66	0.56	25	75	0.67
8	38	70	0.52	19	85	0.81
9	30	72	0.60	13	86	0.84
10*	29	69	0.56	8	66	0.63
11*	29	51	0.31	8	44	0.39
12*	22	48	0.33	8	54	0.50
Average	28	68	0.55	21	74	0.68

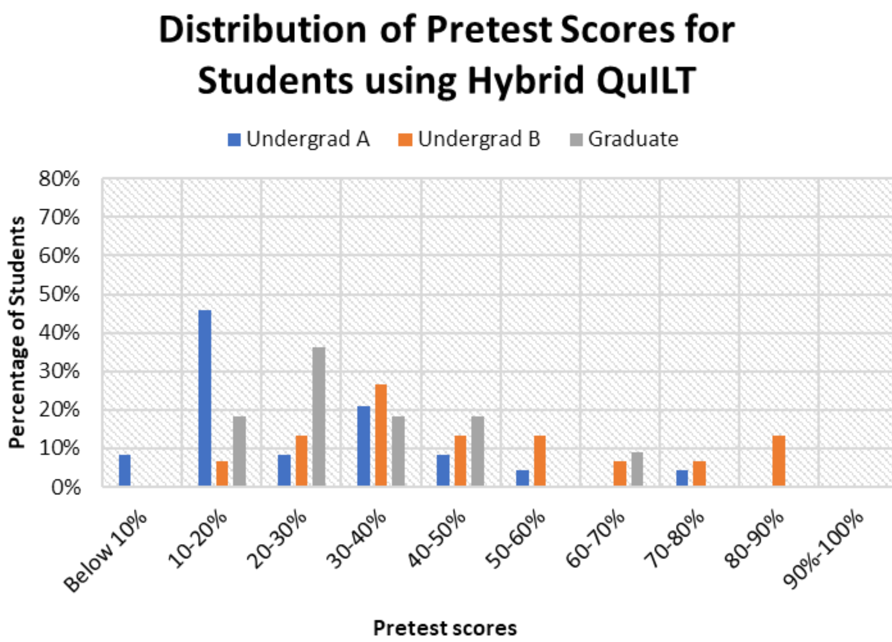


Figure 6.9 Bar graph depicting the distribution of student pretest scores for each hybrid QuILT group.

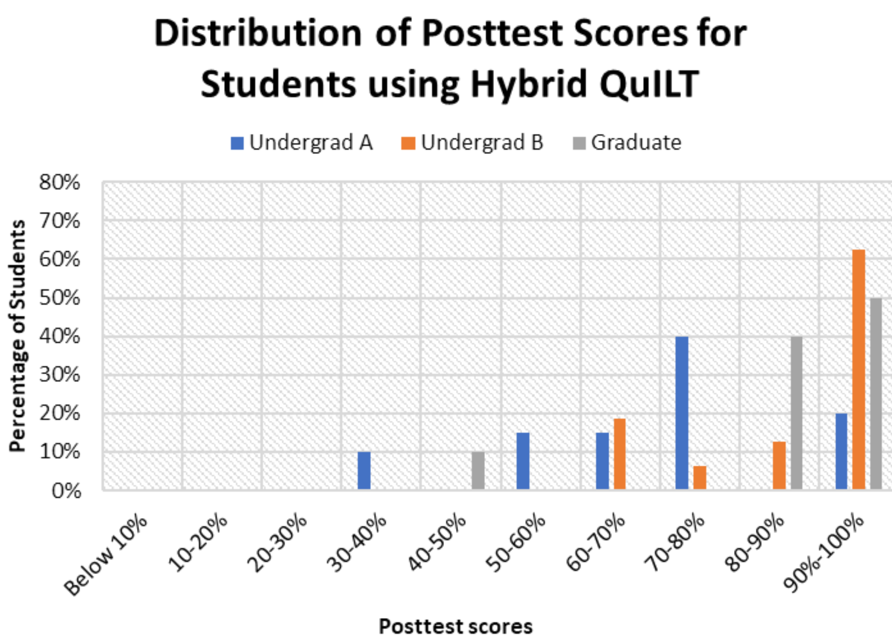


Figure 6.10 Bar graph depicting the distribution of student posttest scores in each hybrid QuILT group.

6.5 RESULTS AND DISCUSSION

Tables 6.1 and 6.2 show percentages of undergraduates and graduate students who correctly answered questions on the MZI pre/posttests before and after engaging with the hybrid QuILT. Normalized gains and effect sizes (Cohen's d) are shown for each class for each question. Table 6.2 represents the same data set as in Table 6.1 but after averaging over the sub-parts of each question. Table 6.3 shows data for (comparison with Table 6.2) mostly from Ref. [93] (although the data for the last few questions have not been published–see caption of Table 6.3) for the pre/posttests administered to undergraduate and graduate students before and after the conceptual MZI QuILT at the same large research university.

6.5.1 Comparison of pre/posttest performance of different groups that learned from the hybrid MZI QuILT

Tables 6.1 and 6.2 show that the graduate students and both groups of undergraduate students performed poorly on the pretest after traditional instruction but the posttest performance after working on the hybrid QuILT was good on most questions for the graduate students and undergraduate group B. However, comparison of undergraduate groups A and B shows that for both the pretest and the posttest, group B performed significantly better on most test items. In particular, only Q1-3, which address more basic concepts (no polarizers are involved so the Hilbert space is two-dimensional) have similar posttest scores in both undergraduate groups A and B (see Table 6.2). This suggests that the hybrid QuILT was effective at helping students learn these concepts.

In contrast, Table 6.2 shows that Q4-6, 8-12 have considerably higher posttest scores for group B, which tended to also perform better on the pretest. In the hybrid QuILT, these questions covered concepts and MZI arrangements involving higher mathematical rigor than Q1-3 (four dimensional Hilbert space involving product space of both path and polarization). Given that these two classes were taught at the same university in subsequent years, the population can be considered comparable in prior mathematical knowledge. One possible reason for the differences between these groups may likely be the difference in the pretest scores, i.e., how much the students had learned about these concepts after traditional instruction in these two courses which were taught by different instructors. In particular, undergraduate students in group A had very low pretest scores on the later questions before they engaged with the hybrid QuILT. This may be due to how the course instructor for undergraduate group A taught this material, how much time the instructor devoted to this topic before students took the pretest and potentially how this material was incentivized. We note that the pretest scores are very low on some of the questions even for the graduate students (see Table 6.2), but they still managed to perform significantly better than undergraduate group A and the graduate students performed comparable to undergraduate group B (which generally had higher pretest scores on later questions than graduate students).

One possible hypothesis for this difference between the average posttest performance of graduate students and undergraduate students in group A (see Table 6.2) despite both groups having poor pretest performance is that the graduate students on average may have better quantitative facility than the undergraduates and this advantage may reduce their cognitive load while learning from the hybrid MZI QuILT despite having low level of initial physics knowledge of the MZI (as inferred from the pretest performance). In particular, since the undergraduate quantum mechanics course is mandatory for all undergraduates whether they are graduate school bound or not, there is a greater diversity in students' quantitative proficiency in the undergraduate course than in the graduate course. Since students' working memory while learning from the hybrid QuILT is limited, if students have both limited conceptual and quantitative facility with the hybrid QuILT content, integration of conceptual and quantitative understanding while learning from the QuILT may cause cognitive overload and leave few cognitive resources for meta-cognition. It is possible that graduate students' poor initial conceptual understanding of the MZI as manifested by their pretest scores did not increase the cognitive load as much as the undergraduate students in group A since graduate students on average had better quantitative facility which can reduce cognitive load while learning from the hybrid QuILT that integrates conceptual and quantitative understanding and leave more cognitive resources for conceptual reasoning and sense-making. In fact, Figures 6.9 and 6.10 show bar graphs of the percentages of students for the three student groups that engaged with the hybrid QuILT. These figures show that while both the undergraduate group A and some graduate students performed poorly on pretest (Fig. 6.9), the pretest scores of many students in undergraduate group A is very low after traditional instruction (this is the group that did not improve significantly on the posttest as shown in Fig. 6.10).

Synthesizing these different comparisons and keeping in mind Table 6.2 and Figures 6.9 and 6.10 (which show that the pretest performance of undergraduate group A is worst followed by graduate students and then undergraduate group B but on the posttest, the graduate student performance is comparable to undergraduate group B with the undergraduate group A performing worst), we hypothesize the possible reasons for two trends. One trend concerns prior mathematical preparation as it pertains to making appropriate math-physics connections and learning new physics concepts in a math-rich context. On average, graduate students at the same university can typically be considered more experienced in applying advanced mathematical skills to physics contexts and are more comfortable changing between and connecting different representations. This is in contrast to upper-level undergraduate students only half of whom are typically graduate school bound. The difference may manifest in graduate students not having as much cognitive overload (as undergraduate group A) when using mathematical representations to learn physics concepts even if their initial physics knowledge of these concepts was not very good as evidenced by their low pretest scores in Table 6.2 and Fig. 6.9. In the case of the MZI, the more mathematically rigorous concepts involved calculations concerning a four-dimensional Hilbert space. On the other hand, undergraduate student group B may have benefited from the hybrid QuILT as much as the graduate students, as evidenced by their posttest performance since they had the best conceptual physics knowledge of these concepts out of the three groups as evidenced by their pretest scores (see Table 6.2 and Fig. 6.9) which may have reduced their cognitive load when engaging with mathematically rigorous concepts and making conceptual inferences from them.

6.5.2 Comparison of pre/posttest performance of graduate students that learned from the hybrid or conceptual MZI QuILT

A comparison of Tables 6.2 and 6.3 shows that both groups of graduate students performed somewhat similarly on average on the pretests although there are some variations across questions (e.g., the hybrid QuILT group's performance on Q1-3 suggests their lecture experience had them better prepared for the more basic concepts of the MZI than their conceptual QuILT counterparts, but their performance on Q6-12 suggests that the opposite is true for the more complex situations). On the posttest, however, the hybrid QuILT group performed, at worst, roughly the same as, and in most cases, considerably better than their conceptual QuILT counterpart. One possible explanation is that, for the graduate students, a population that is likely to have higher quantitative facility at least in the context of physics, the integrated conceptual and quantitative MZI QuILT improves student performance on conceptual questions on many of the concepts compared to the conceptual MZI QuILT.

6.5.3 Comparison of pre/posttest performance of undergraduates that learned from the hybrid or conceptual MZI QuILT

With some variations by question, the hybrid QuILT undergraduate group A (see Table 6.2) on average performed somewhat similarly to the conceptual QuILT group on the pretest (see Tables 6.2 and 6.3). There were clear trends on which conceptual issues pertaining to the MZI exhibited better pretest performance. However on the posttest, group A performed better on Q1-3, while performing worse on Q7-11. For example, question 3 focuses on the role of beam-splitter 2 (BS2) and how it affects interference of single photons. In particular, this question investigates whether students understand how removing or inserting beam-splitter BS2 will change the probability of the single photons arriving at each detector D1 or D2. An integrated conceptual and quantitative inquiry-based sequences involving a two dimensional Hilbert space were designed to provide scaffolding support to have students contemplate the role of BS2 and whether interference is observed for single photons without BS2. The posttest performance of all student groups (graduate students and undergraduate groups A and B) after engaging with the hybrid QuILT is close to perfect whereas both graduate and undergraduate students averaged 79% after engaging with the conceptual QuILT (see Tables 6.2 and 6.3).

One possible hypothesis for why undergraduate student group A in Table 6.2 performed well on Q1-3 but not on Q7-11 attributes this difference across questions on the posttest to the mathematical facilities of group A (especially in the light of the fact that they had poor conceptual understanding of the underlying concepts as reflected by the low pretest scores) and the fact that the increased mathematical rigor in the hybrid QuILT may have caused a cognitive overload for students particularly for the questions involving polarizers that involves product states of path and polarization. In particular, concepts involved in Q1-3 require a two dimensional Hilbert space (only photon path states through the MZI are relevant since polarizers are not present). On these questions, undergraduates in Group A appear to have benefitted more from the hybrid QuILT as reflected by their posttest performance. However, for Q7-11 on the posttest, which involve the four-dimensional Hilbert space (since both photon path states and polarization states must be taken into account to understand the outcomes of the experiment) their performance is poor.

In contrast, the undergraduate group B which engaged with the hybrid QuILT exhibited better pretest performance than the undergraduates who engaged with the conceptual QuILT. This is likely an instructor effect with the instructor of the undergraduate group B preparing and incentivizing students better than the instructor of the undergraduate conceptual QuILT group. Moreover, these undergraduate students in group B outperformed all other groups on the conceptual posttest including those who engaged with the conceptual QuILT.

We note that question (4) on the posttest evaluates student understanding of the role of additional detectors inserted into one of the paths of the MZI. In particular, it investigates student understanding of how inserting an additional detector in the U path of the MZI would affect the interference at the detectors D1 and D2. Students need to reason that an additional detector would collapse the state of the photon to the U or L path state (instead of the single photon state being a superposition of the U and L path states) and how the collapse of the photon state to the U or L path state causes the detectors D1 or D2 after BS2 to click with equal probability and destroys the interference at the detectors. This type of situation is covered in the conceptual QuILT but is not covered in the hybrid MZI QuILT, although students had learned about the role of detectors D1 and D2 after BS2. Table 6.2 shows that on the posttest, graduate students and undergraduates in group B who engaged with the hybrid QuILT performed comparably to the graduate and undergraduate students in the conceptual QuILT group. This is encouraging since it suggests that students were able to transfer their learning about the role of detectors from those after BS2 (photo-detectors D1 and D2) to a detector in the U path of the MZI. For example, we believe this is a farther transfer compared to the situation in question 10 on the posttest in which students had worked through a situation in which the polarizer right before detector D1 was a vertical polarizer (instead of a horizontal polarizer).

6.6 DISCUSSION AND SUMMARY

We use the "Integrating Conceptual and Quantitative Understanding In Physics" or "ICQUIP" framework to develop, validate and evaluate a Quantum Interactive Learning Tutorial (QuILT) which incorporates mathematical rigor while focusing on helping students develop expertise, i.e., a good conceptual understanding of quantum optics using a Mach Zehnder Interferometer with single photons and polarizers. The "ICQUIP" framework posits that appropriate integration of conceptual and quantitative aspects of physics in teaching and assessing student learning is central for effective instruction, advancing students along the expertise spectrum and equipping them with adequate level of mastery within the context of a physics course. Constructing a conceptual reasoning chain without equations can be more difficult than learning to reason with quantitative tools by constraint satisfaction. The framework also emphasizes that the instructional design should provide appropriate scaffolding support to students commensurate with their prior knowledge and skills to integrate conceptual and quantitative understanding, learn physics concepts and develop their problem solving, reasoning and meta-cognitive skills. In other words, if the level of math-physics connection (or conceptual and quantitative connection) is not appropriate, use of quantitative tools in courses can increase students' cognitive load to the extent that very little cognitive resources may be available for drawing conceptual inferences from them. These issues are critical due to the limited capacity of working memory. In other words, in order to learn physics and build a robust knowledge structure with quantitative tools [23], students must be given opportunities to interpret symbolic equations correctly and be able to draw conceptual inferences from them. This implies that students must be given support to not treat quantitative problem solving merely as a mathematical exercise but as an opportunity for sense making, learning physics concepts and developing expertise. This requires that students are provided scaffolding to engage in effective problem solving strategies. Through integration of appropriate levels of mathematics and physics and expecting students to learn to reason by drawing conceptual inferences from quantitative problem solving in order to perform well in the course, physics learning and expertise development can, in general, be enhanced significantly.

The hybrid MZI QuILT uses an approach consistent with the ICQUIP framework and integrates conceptual and quantitative aspects of MZI experiments to develop students' expertise and conceptual understanding of physics. We compared upper-level undergraduate and graduate students' performance on conceptual questions after engaging with this hybrid QuILT with a conceptual QuILT [93] focusing on the same topics in which quantitative tools were not employed. Both versions of the QuILT use a guided inquiry-based approach to learning and are based on research on student difficulties in learning these challenging concepts as well as a cognitive task analysis from an expert perspective. We find that physics graduate students' posttest performance on conceptual questions after engaging with the hybrid QuILT was generally better than their performance after engaging with the conceptual QuILT. For undergraduate students, the findings were mixed. One group of undergraduates, which had reasonable pretest scores after traditional lecture-based instruction on these topics and which engaged with the hybrid QuILT after the pretest, outperformed the undergraduates who engaged with the conceptual QuILT on the posttest, which was completely conceptual. On the other hand, another group of undergraduates, which had very low average pretest score after traditional lecture-based instruction on these topics and which engaged with the hybrid QuILT after the pretest, had good posttest performance on some conceptual questions, especially those pertaining to a two-dimensional Hilbert space involving only path states of the single photons through the MZI. However, their posttest performance on many of the other conceptual posttest questions was worse than the undergraduates who used the conceptual QuILT.

One possible interpretation of these findings consistent with the ICQUIP framework is that integration of conceptual and quantitative aspects of physics should be commensurate with students' prior knowledge of physics and mathematics involved so that students do not experience cognitive overload while engaging with such a learning tool striving to develop a good grasp of physics concepts. In the undergraduate course in which students did not benefit as much from the hybrid QuILT that focused on integration of conceptual and quantitative understanding to help students learn physics concepts, their pretest performance suggests that the traditional instruction may not have sufficiently given a “first coat” and prepared students with requisite physics concepts to engage with the hybrid QuILT. Since physics majors in the mandatory undergraduate quantum mechanics course come with diverse physics and mathematics backgrounds, the hybrid QuILT may have caused cognitive overload at least for some students (on topics in which their conceptual posttest performance is not good) so that they could not benefit from integrated conceptual and quantitative learning sequences. In other words, integration of conceptual and quantitative understanding in physics must adequately build on students’ prior knowledge to avoid cognitive overload and help students develop expertise.

In summary, conceptual and quantitative aspects of physics learning should be integrated appropriately in order to help students develop physics expertise at all levels. By incorporating mathematical rigor in the hybrid MZI QuILT, we aimed to improve students’ conceptual understanding of the challenging single photon quantum mechanics experiments in the context of a MZI as measured by the conceptual posttest questions. By comparing to performance on conceptual pretest and posttest, we find that integrating conceptual and quantitative aspects of the MZI with single photons in the hybrid MZI QuILT provided opportunity for more effective learning for graduate students and undergraduates who had an adequate first coat of conceptual understanding of the MZI experiments when compared to students who engaged with the conceptual MZI QUILT. On the other hand, undergraduates who had very low pretest scores before engaging with the hybrid QuILT exhibited similar or worse conceptual learning than those who engaged with the conceptual QuILT. One possible hypothesis for the significantly better posttest performance of graduate students compared to the undergraduates, both of whom engaged with the hybrid QuILT and performed poorly on the pretest, is that the graduate students with more experience using advanced math in the physics context were able to more consistently and effectively benefit from the mathematical representations of concepts in the hybrid QuILT and did not experience cognitive overload despite having low level of conceptual understanding of the MZI with single photons are manifested by the pretest scores. Thus, adequate prior physics and mathematical facility above a certain threshold is necessary for students to be in the optimal adaptability corridor and engage effectively with the hybrid QuILT that integrates conceptual and quantitative understanding of physics.

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6.9 CHAPTER APPENDIX: MACH-ZEHNDER INTERFEROMETER (MZI)

POSTTEST

The setup for the ideal Mach-Zehnder Interferometer (MZI) shown below in Figure 1 is as follows:

- The photons originate from a monochromatic coherent point source. (Note: Experimentally, a source can only emit nearly monochromatic photons such that there is a very small range of wavelengths coming from the source. Here, we assume that the photons have negligible "spread" in energy.)
- Assume that the photons propagating through both the U and L paths travel the same distance in vacuum to reach each detector.
- All angles of incidence are 45° with respect to the normal to the surface.
- For simplicity, we will assume that a photon can only reflect from one of the two surfaces of the identical half-silvered mirrors (beam splitters) BS1 and BS2 because of an anti-reflection coating on one of the surfaces.
- Assume that beam splitters BS1 and BS2 are infinitesimally thin so that there is no phase shift when a photon propagates through them.
- The phase shifter is ideal and non-reflective.
- Ignore the effect of polarization of the photons due to reflection by the beam splitters or mirrors.
- The photo-detectors D1 and D2 are point detectors located symmetrically with respect to the other components of the MZI as shown.
- All photo-detectors are ideal and 100% efficient.
- Polarizers do not introduce phase shifts.
- All measurements are ideal projective measurements.

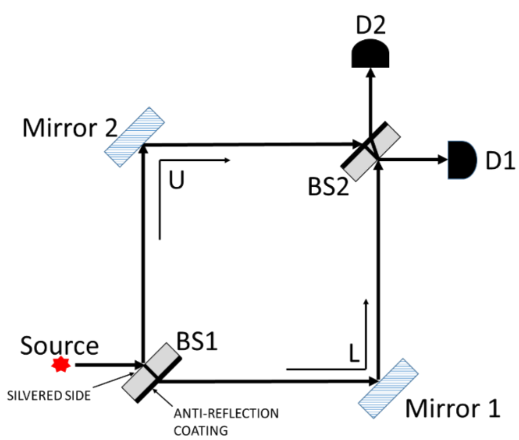


Figure 1

For all of the following questions, assume that:

- The single photons are emitted from the source in a highly collimated stream, i.e., the width of the transverse Gaussian profile of each photon is negligible.
- A very large number (N) of single photons are emitted from the source one at a time and pass through beam splitter BS1.

1. Consider the following statement about single photons emitted from the source in Figure 1:
    - If the source emits N photons one at a time, the number of photons reaching detectors D1 and D2 will be $N/2$ each.

    Explain why you agree or disagree with this statement.

2. Consider the following conversation between Student 1 and Student 2:

    - Student 1: The beam splitter BS1 causes the photon to split into two parts and the energy of the incoming photon is also split in half. Each photon with half of the energy of the incoming photon travels along the U and L paths of the MZI and produces interference at detectors D1 and D2.
    - Student 2: If we send one photon at a time through the MZI, there is no way to observe interference in the detectors D1 and D2. Interference is due to the superposition of waves from the U and L paths. A single photon must choose either the U or the L path.

    Do you agree with Student 1, Student 2, both, or neither? Explain your reasoning.

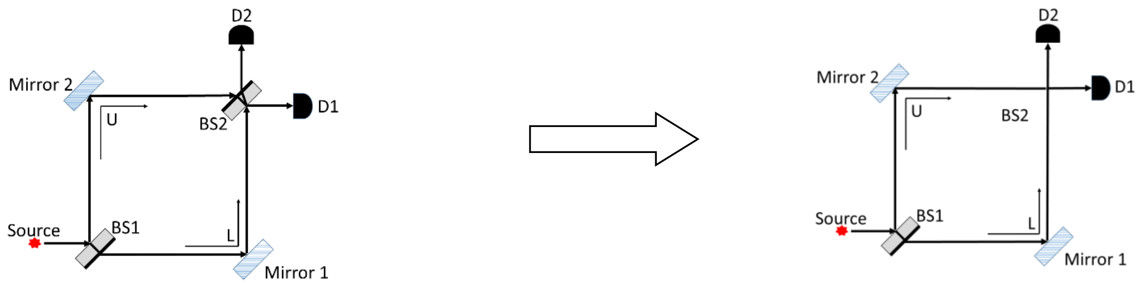


Figure 2

3a. Suppose we remove BS2 from the MZI setup as shown in Figure 2 above. How does the probability that detector D1 or D2 will register a photon in this case differ from the case when BS2 is present as in Figure 1? Explain your reasoning.

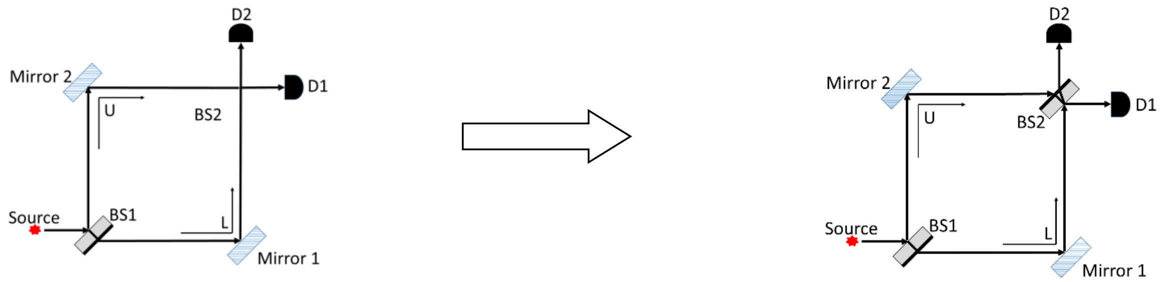


Figure 3

3b. Suppose we have an MZI setup initially without BS2. If we suddenly insert BS2 after the photon enters BS1 but before it reaches the point where BS2 is inserted (see Figure 3 above), with what probabilities do detectors D1 and D2 register the photon? Explain your reasoning. Assume that the situation after BS2 is inserted is identical to Figure 1.

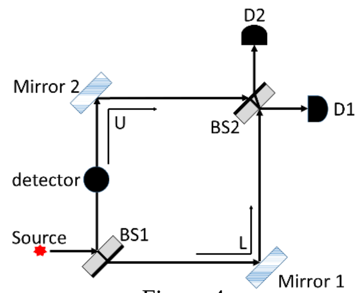


Figure 4

4. Suppose we modify the set up shown in Figure 1 and insert a photo-detector into the upper path between BS1 and mirror 2 as shown in Figure 4.
   a) What is the fraction of single photons emitted by the source that reach each detector D1 and D2? Explain your reasoning.

   b) If you place a phase shifter in the L path and change its thickness gradually to change the path length difference between the U and L paths, how would the phase shifter affect the fraction of photons arriving at detectors D1 and D2? Explain your reasoning.

   c) If there is interference displayed in part 5b) by any photons at detector D1, write down the percentage of the photons emitted by the source that display interference. You must explain

For all of the following questions, assume that the single photon source emits photons that are polarized at +45°.

6. Consider the following statement about a source emitting +45° polarized single photons:
   - If we place additional polarizers in the paths of the MZI, the polarizers will absorb some photons and they will not arrive at the detectors. However, the polarizers will not affect whether interference is displayed at the detectors.

   Explain why you agree or disagree with the statement

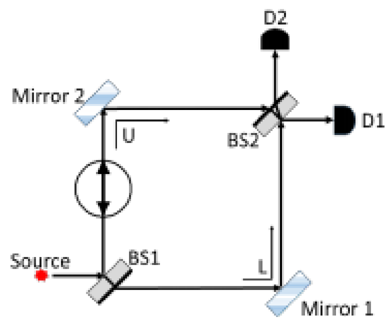


Figure 5

7. You modify the set up shown in Figure 1 by inserting a polarizer with a vertical polarization axis as shown in Figure 5.
    a) What is the fraction of single photons emitted by the source that reach each detector D1 and D2? Explain your reasoning.

    b) If you place a phase shifter in the U path and change its thickness gradually to change the phase difference between the U and L paths, how would the phase shifter affect the fraction of photons arriving at detectors D1 and D2? Explain your reasoning.

    c) If there is interference displayed by any photons in part 7b) at detector D1, write down the percentage of the photons emitted by the source that display interference. You must explain your reasoning.

    d) Describe in detail what you would observe at the detectors D1 and D2 in Figure 5 above and how this situation will differ from the case in Figure 1 in which there is no polarizer in path U. Assume both in Figure 1 and Figure 5 that the source emits single photons that are polarized at 45°.

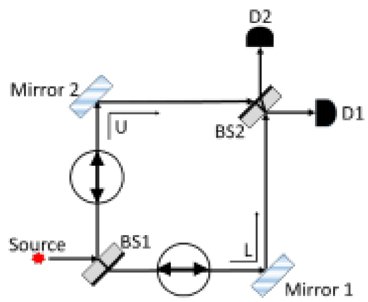


Figure 6

8. You modify the set up shown in Figure 1 and insert polarizer 1 with a vertical polarization axis (between BS1 and mirror 2) and polarizer 2 with a horizontal polarization axis (between BS1 and mirror 1) in the U and L paths as shown in Figure 6.
   a) What is the fraction of single photons emitted by the source that reach each detector D1 and D2? Explain your reasoning.

   b) If you place a phase shifter in the U path and change its thickness gradually to change the phase difference between the U and L paths, how would the phase shifter affect the fraction of photons arriving at detectors D1 and D2? Explain your reasoning.

   c) If there is interference displayed by any photons in part 8b) at detector D1, write down the percentage of the photons emitted by the source that display interference. You must explain your reasoning.

   d) Describe in detail what you would observe at the detectors D1 and D2 in Figure 6 above and how this situation will differ from the case in Figure 5 in which only polarizer 1 was present (as in question 7). Explain your reasoning.

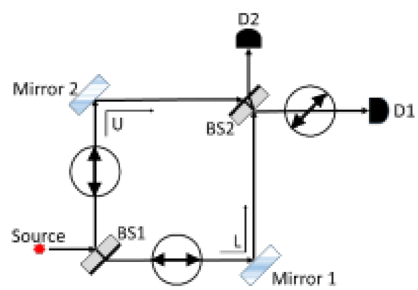


Figure 7

9. You start with the set up shown in Figure 6 with polarizer 1 with a vertical polarization axis and polarizer 2 with a horizontal polarization axis inserted in the U and L paths, respectively. You modify the set up and insert polarizer 3 with a +45° polarization axis between BS2 and detector D1 (see Figure 7).
   a) What is the fraction of single photons emitted by the source that reach each detector D1 and D2? Explain your reasoning.

   b) If you place a phase shifter in the U path and change its thickness gradually to change the phase difference between the U and L paths, how would the phase shifter affect the fraction of photons arriving at detectors D1 and D2? Explain your reasoning.

   c) If there is interference displayed by any photons in part 9b) at detector D1, write down the percentage of the photons emitted by the source that display interference. You must explain your reasoning.

   d) Describe in detail what you would observe at the detectors D1 and D2 in Figure 7 above and how this situation will differ from the case in Figure 6 in which polarizer 3 was not present (as in question 8). Explain your reasoning.

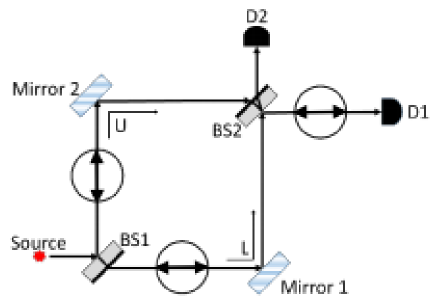


Figure 8

10. You start with the set up shown in Figure 6 with polarizer 1 with a vertical polarization axis and polarizer 2 with a horizontal polarization axis inserted in the U and L paths, respectively. You modify the set up and insert polarizer 3 with a horizontal polarization axis between BS2 and the detector D1 (see Figure 8).
    a) What is the fraction of single photons emitted by the source that reach each detector D1 and D2? Explain your reasoning.

    b) If you place a phase shifter in the U path and change its thickness gradually to change the phase difference between the U and L paths, how would the phase shifter affect the fraction of photons arriving at detectors D1 and D2? Explain your reasoning.

    c) If there is interference displayed by any photons in part 10b) at detector D1, write down the percentage of the photons emitted by the source that display interference. You must explain your reasoning.

    d) Describe in detail what you would observe at the detectors D1 and D2 in Figure 8 above and how this situation will differ from the case in Figure 6 in which polarizer 3 was not present (as in question 8). Explain your reasoning.

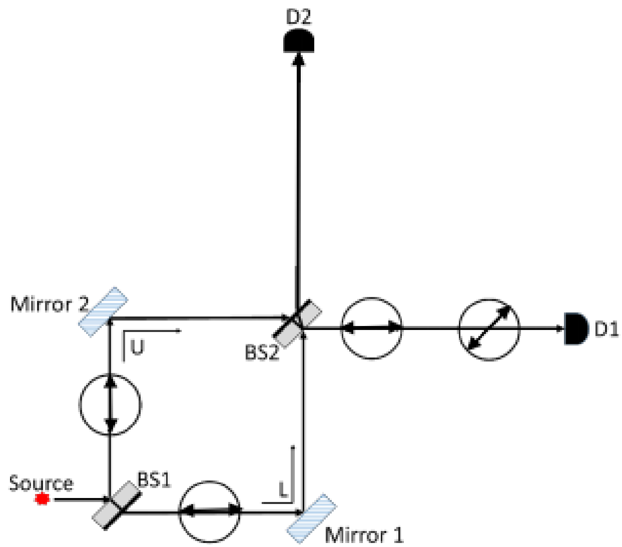


Figure 9

11. You set up an MZI as shown in Figure 9, inserting polarizer 1 with a vertical polarization axis and polarizer 2 with a horizontal polarization axis in the U and L paths, respectively. You also insert polarizer 3 with a horizontal polarization axis and polarizer 4 with a 45° polarization axis between BS2 and detector D1 (see Figure 9).
    a) What is the fraction of single photons emitted by the source that reach each detector D1 and D2? Explain your reasoning.

    b) If you place a phase shifter in the U path and change its thickness gradually to change the phase difference between the U and L paths, how would the phase shifter affect the fraction of photons arriving at detectors D1 and D2? Explain your reasoning.

    c) If there is interference displayed by any photons in part 11b) at detector D1, write down the percentage of the photons emitted by the source that display interference. You must explain your reasoning.

    d) How does what you observe at the detectors D1 and D2 in Figure 9 above compare with the situation in which polarizer 3 was not present?

12. Describe an experiment using a Mach-Zehnder Interferometer in which you could distinguish between a source emitting unpolarized photons and a source emitting +45° polarized photons.

7.0 FUTURE DIRECTIONS

In this thesis, I discussed the development, validations and implementation of multiple instructional tools to help students learn upper-level quantum mechanics. The use of robust clicker question sequences (CQS) pertaining to many quantum mechanics concepts was found to be effectiveness in improving students' conceptual understanding on relevant concepts. However, many of these sequences can still be iterated, refined, and improved particularly after implementing them in classes at other universities and colleges. Some common student difficulties still have room to be addressed in a more impactful way.

The findings in this thesis have implications for improving teaching and learning of not only upper-level quantum mechanics, but also for developing learning tools for other introductory and advanced courses. Here the framework for the development, validation and implementation of a CQS has been applied to an upper-level quantum mechanics course. The effectiveness of this framework to helping students learn physics in other courses, such as introductory physics, should be investigated in the future. Additionally, a number of CQSs have been developed for other topics in upper-level quantum mechanics. Some of these can be found in Appendix B. While preliminary data has been gathered for most of these CQSs, not only should those data be analyzed in the future, the CQSs should be refined and iterated by researchers based upon data analysis and further implemented and evaluated in the refined form.

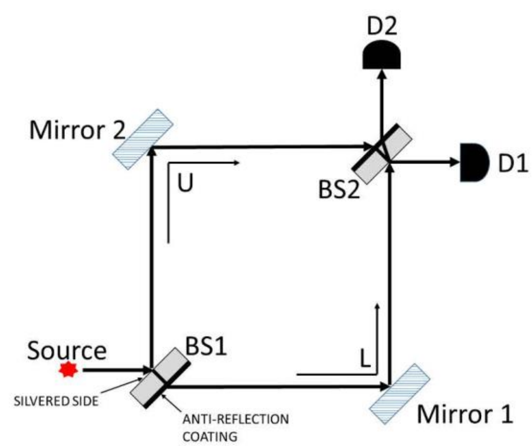
APPENDIX A: MACH-ZEHNDER INTERFEROMETER HYBRID QUANTITATIVE-QUALITATIVE QuILT

A.1 HYBRID QuILT SECTION WITHOUT POLARIZERS

Understanding the Mach-Zehnder Interferometer (MZI) with Single Photons: Homework

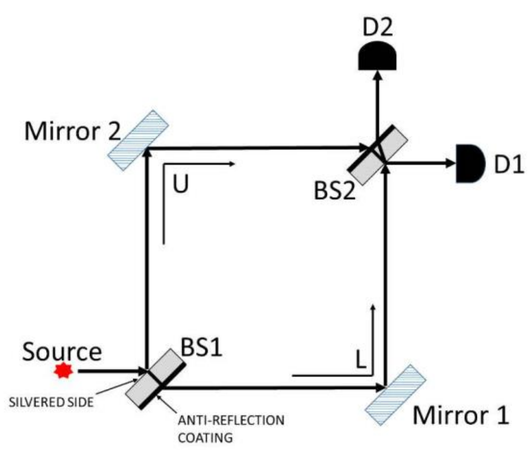
The goal of this homework is to use a simplified ideal version of MZI to help you:

- **Connect qualitative understanding of the MZI with a simple mathematical model**
- **After choosing a basis, you will:**
  - **A. Determine the matrix representations of quantum mechanical operators that correspond to beam splitter 1 and beam splitter 2**
  - **B. Determine the matrix representation of the quantum mechanical operator that corresponds to the mirrors**
  - **C. Find the action of the beam splitters BS1 and BS2 on an input state and the probability of a detector D1 or D2 "clicking"**
  - **D. Determine the matrix representation of a quantum mechanical operator that corresponds to a phase shifter (e.g., a glass piece of a certain thickness inserted into one of the paths of the MZI)**
  - **E. Find probabilities of detectors "clicking" after a phase shifter is inserted and acquire intermediate interference at detectors D1 and D2 (neither fully constructive nor fully destructive)**
  - **F. Verify that the matrix representation of the quantum mechanical time-evolution operators corresponding to beam splitter 1, beam splitter 2, mirrors, and phase shifter evolve the state of the system in time and are unitary operators which preserve the norm of the physical state**



The setup for the ideal Mach-Zehnder Interferometer (MZI) shown below is as follows:

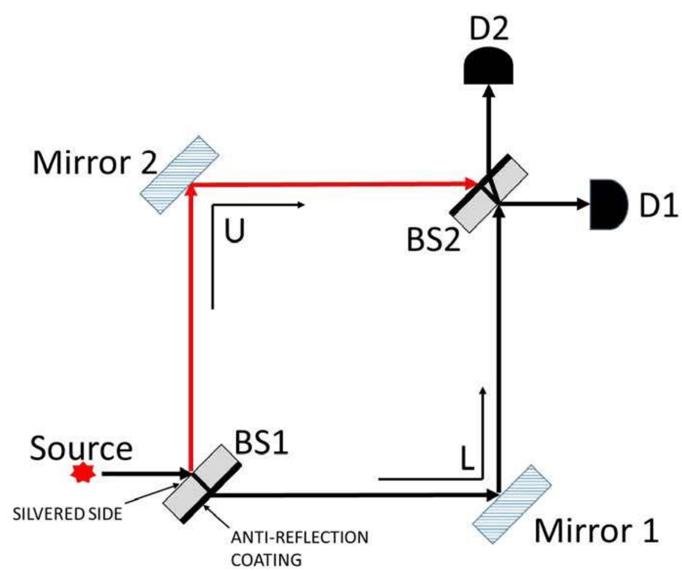
- The photons originate from a monochromatic coherent point source. (Note: Experimentally, a source can only emit nearly monochromatic photons such that there is a very small range of wavelengths coming from the source. Here, we assume that the photons have negligible "spread" in energy.)
- Assume that the photons propagating through both the U and L paths travel the same distance in vacuum to reach each detector.
- All angles of incidence are 45° with respect to the normal to the surface.
- For simplicity, we will assume that a photon can only reflect from one of the two surfaces of the identical half-silvered mirrors (beam splitters) BS1 and BS2 because of an anti-reflection coating on one of the surfaces.
- Assume that beam splitters BS1 and BS2 are infinitesimally thin so that there is no phase shift when a photon propagates through them.
- The phase shifter is ideal and non-reflective.
- Ignore the effect of polarization of the photons due to reflection by the beam splitters or mirrors.
- The photo-detectors D1 and D2 are point detectors located symmetrically with respect to the other components of the MZI as shown.
- All photo-detectors are ideal and 100% efficient.
- Polarizers do not introduce phase shifts.
- All measurements are ideal projective measurements.
- "Which-path" information is known when each detector D1 and D2 shown below can only project the component of the photon state along the U path or the L path. "Which-path" information is unknown when each detector D1 and D2 can project both the U and L components of the photon state.
- For the entire tutorial, assume that a large number of photons (N) are sent one at a time.



2

Before we begin, we will make a few assumptions and observations:

- The beam splitters are 50/50 splitters, meaning that a measurement of the photon position immediately after it exits the beam splitter BS1 would yield an outcome such that the photon is either in the upper path or the lower path with 50% probability.
- The silvered side of the beam splitter is the point of reflection. No reflection occurs at the air-glass interface (the bold side of the beam splitter), due to anti-reflection coatings.
- From here on, assume that the thickness of the beam splitters is negligible so the phase shift introduced by the propagation of light through the beam splitters is zero ($\varphi_{BS} = 0$).
- No relative phase shift between the $|U\rangle$ and $|L\rangle$ path states is introduced when a photon propagates through vacuum because the photon travels the same distance in vacuum along each of the U and L paths.
- In all of the matrix representations of the operators, in a given basis, we will simplify the "≐" sign which means "is represented in a given basis by" with "=" for convenience.
- To differentiate between the upper and lower path inside the MZI, the upper path U is marked in RED and the lower path L is marked in BLACK.



3

A. Determining the matrix representations of the quantum mechanical operators that correspond to Beam Splitter 1 (BS1) and Beam Splitter 2 (BS2)

In a simplified quantum mechanical model of a photon state which accounts for the two paths U and L, a single photon traveling through the MZI can be considered to be a two state quantum system.

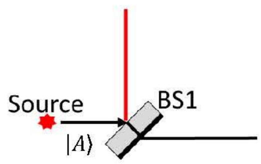


Figure 1.a : photon initially in $|A\rangle$ path state

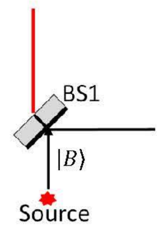


Figure 1.b: photon initially in $|B\rangle$ path state

- Let's consider **BS1**. Note that in Figure 1.a and Figure 1.b, depending on the position of the source, a photon can travel along different paths before it enters BS1. We will call these initial path states $|A\rangle$ and $|B\rangle$.
- Let's choose a basis in which we denote the state of the photon from the source towards BS1 along path state $|A\rangle = \binom{1}{0}$ as shown in Figure 1.a and denote the state along the path state $|B\rangle = \binom{0}{1}$ as shown in Figure 1.b.
- Inside the MZI, let's choose a basis in which we denote the state of the photon in the upper state (RED path), by $|U\rangle = \binom{1}{0}$ and denote the state along the lower path (BLACK path), by lower state $|L\rangle = \binom{0}{1}$.
- After exiting BS1, the quantum mechanical state of the photon is in an equal superposition of the upper and lower states (since BS1 is a 50/50 beam splitter).
- If a measurement of the photon's position is made immediately after BS1 by a photo-detector, the measurement would yield the photon either in the RED path, denoted by upper state $|U\rangle = \binom{1}{0}$, or the BLACK path, denoted by lower state $|L\rangle = \binom{0}{1}$.

Here is a summary of the phase shifts from the MZI warm-up. Use this table to find the phase shifts for the photon that enters BS1 and goes into a state which is an equal superposition of the U and L states. Knowing the phase shifts will help us determine the superposition state of the photon after exiting BS1 and the operator matrix for BS1.

Table 1

	Initially in medium with lower n	Initially in medium with higher n
Reflection at interface	Phase shift of π	No phase shift
Transmission at interface	No phase shift	No phase shift
Propagation through a medium	Phase shift φ depends on thickness and refractive index n of the medium	

- Since there are two linearly independent states of the photon in this simplified model, i.e., $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$, the Hilbert space is two dimensional.
- Any operator in a two dimensional Hilbert space can be represented by a 2×2 matrix in the chosen basis.
- We can think of the beam splitters and mirrors as quantum mechanical operators which act on the photon state and change it at various times during its propagation through the MZI.

The **BS1** operator acts on a photon in an initial state (either $|A\rangle$ or $|B\rangle$ depending on the location of the source) and puts it into an equal superposition of the upper and lower states. We will denote the quantum mechanical operator corresponding to BS1 as [BS1].

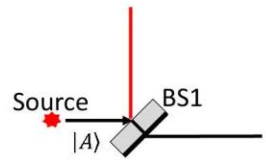


Figure 1.a: photon initially in $|A\rangle$ path state

1. Consider the following statements from three students about the effect of operator [BS1] on the initial photon state $|A\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ shown in Figure 1.a

   - Student 1: $[\text{BS1}]\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\right]$ since the operator [BS1] puts the photon state into an equal superposition of $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$.

   - Student 2: No, $[\text{BS1}]\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix}\right]$ because there is a phase shift of π for the part that passes through BS1 and $e^{i\pi} = -1$.

   - Student 3: No. $[\text{BS1}]\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\left[-\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\right]$ since there is a phase shift of π for the part that reflects and no phase shift for the part that passes through BS1.

   Which students, if any, do you agree with and why? (Hint: look at Table 1)

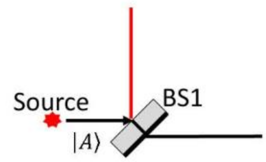


Figure 1.a: photon initially in $|A\rangle$ path state

The action of the operator [BS1] on the photon in the initial state $|A\rangle = \binom{1}{0}$ as shown in Figure 1.a should be

$$[\text{BS1}]\,|A\rangle = [\text{BS1}]\binom{1}{0} = \frac{1}{\sqrt{2}}\left[-\binom{1}{0} + \binom{0}{1}\right] = \frac{1}{\sqrt{2}}\binom{-1}{1} \tag{1}$$

The $\frac{1}{\sqrt{2}}$ ensures that after the photon exits BS1, there is a 50% probability that a measurement of the photon's position would yield the photon either in the upper or lower state. Using Table 1, the upper state is multiplied by -1 because of the reflection at the vacuum-BS1 interface (initially in a medium with a lower index of refraction). Thus, the upper state undergoes a phase change of π. Therefore, we multiply the upper state by $e^{i\pi} = -1$. The lower state is transmitted at the vacuum-BS1 interface, so it is not phase shifted (see Table 1).

2. Call the [BS1] matrix in the given basis $\begin{bmatrix} a & b \\ c & d \end{bmatrix}$. Using equation (1) and $[\text{BS1}] = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$, determine the matrix elements a and c.

Now let's determine matrix elements b and d of the operator [BS1].

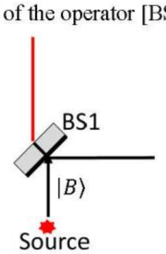


Figure 1.b: photon initially in $|B\rangle$ path state

3. Consider Figure 1.b for which the initial state of the photon before passing through BS1 is $|B\rangle = \binom{0}{1}$. Use Table 1 to find the phase shifts of the upper and lower states immediately after the photon exits BS1.

4. The action of the operator BS1 on the photon in the initial state $|B\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ as shown in Figure 1.b should be

$$[\mathrm{BS1}]|B\rangle = [\mathrm{BS1}]\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\right] \quad (2)$$

Since the upper and lower states are not phase shifted in this case (see Table 1), there are no minus signs. Using equation (2) and $[\mathrm{BS1}] = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$, find the matrix elements b and d of the operator [BS1].

5. Write down the matrix $\begin{bmatrix} a & b \\ c & d \end{bmatrix}$ for the operator [BS1] corresponding to beam splitter 1 in terms of what you found in the preceding questions 1-4.

Now we need to find the matrix representation of the operator [BS2], the quantum mechanical operator corresponding to beam splitter **BS2**, for the two state system for a photon we are considering corresponding to the two possible paths U and L.

- Let's consider **BS2**. Note that in Figure 2.a and Figure 2.b, a photon can travel along different paths before it is registered at detector D1 or detector D2. We will call these final path states $|C\rangle$ and $|D\rangle$.
- Let's choose a basis in which we denote the state of the photon propagating towards detector D1 as path state $|C\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and denote the state of the photon propagating towards detector D2 as the path state $|D\rangle = \begin{pmatrix}0\\1\end{pmatrix}$.

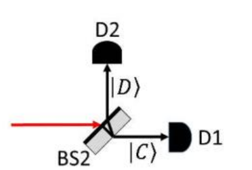


Figure 2.a: Photon enters BS2 via upper path

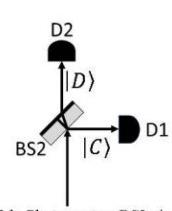


Figure 2.b: Photon enters BS2 via the lower path

6. In Figure 2.a, the photon enters BS2 from the upper path. Use Table 1 to find the phase shifts of the final states after the photon exits BS2.

7. Using the phase shifts identified in the preceding question, what is $[\text{BS2}]\binom{1}{0}=$?

(a) $[\text{BS2}]\binom{1}{0}=\frac{1}{\sqrt{2}}\left[-\binom{1}{0}+\binom{0}{1}\right]$

(b) $[\text{BS2}]\binom{1}{0}=\frac{1}{\sqrt{2}}\left[\binom{1}{0}-\binom{0}{1}\right]$

(c) $[\text{BS2}]\binom{1}{0}=\frac{1}{\sqrt{2}}\left[-\binom{1}{0}-\binom{0}{1}\right]$

(d) $[\text{BS2}]\binom{1}{0}=\frac{1}{\sqrt{2}}\left[\binom{1}{0}+\binom{0}{1}\right]$

8. The correct answer for question 7 is (d), since neither final state $|C\rangle$ nor the final state $|D\rangle$ is phase shifted. Let the operator matrix in the given basis be $[\text{BS2}]=\begin{bmatrix} e & f \\ g & h \end{bmatrix}$. Find the matrix elements e and g using the answer to the preceding question.

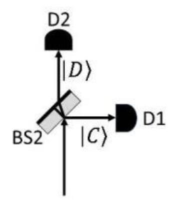


Figure 2.b: Photon enters BS2 via the lower path

9. In Figure 2.b, the photon enters BS2 from the lower path. Use Table 1 to find the phase shifts of the final states after the photon exits BS2.

10. Using the phase shifts identified in the preceding question, what is $[\text{BS2}]\binom{0}{1}=$?

(a) $[\text{BS2}]\binom{0}{1}=\frac{1}{\sqrt{2}}\left[-\binom{1}{0}+\binom{0}{1}\right]$

(b) $[\text{BS2}]\binom{0}{1}=\frac{1}{\sqrt{2}}\left[\binom{1}{0}-\binom{0}{1}\right]$

(c) $[\text{BS2}]\binom{0}{1}=\frac{1}{\sqrt{2}}\left[-\binom{1}{0}-\binom{0}{1}\right]$

(d) $[\text{BS2}]\binom{0}{1}=\frac{1}{\sqrt{2}}\left[\binom{1}{0}+\binom{0}{1}\right]$

11. The correct answer to the preceding question 10 is (a), since the final state C undergoes a phase change of π. Therefore, we multiply the state C by $e^{i\pi} = -1$. The final state D is not phase shifted. Use your answers to the preceding questions to find the matrix elements f and h of the [BS2] matrix.

12. Write down the matrix $\begin{bmatrix} e & f \\ g & h \end{bmatrix}$ for the operator [BS2] corresponding to beam splitter 2 in terms of what you found in the preceding questions.

13. Consider the following conversation between two students:
    - Student A: The matrices we found for the operators corresponding to BS1 and BS2 are [BS1]= $\frac{1}{\sqrt{2}}\begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}$ and [BS2]= $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$. This makes sense because we chose the basis vectors in the order $|U\rangle$, $|L\rangle$ and $|A\rangle$, $|B\rangle$ (see matrix [BS1] below). If the photon is in the initial state $|A\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, after it propagates through BS1, the component of the photon path state in the upper path state $|U\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ undergoes a phase change of π of the upper path state (multiplied by $e^{i\pi} = -1$). Thus the matrix element $\langle A|BS1|U\rangle = -\frac{1}{\sqrt{2}}$ (the $\frac{1}{\sqrt{2}}$ ensures that after the photon exits BS1, there is a 50% probability that a measurement of the photon's position would yield the photon either in the upper or lower state). The remaining photon components do not undergo any phase shift and the corresponding matrix elements are positive.

$$[BS1] = \begin{array}{c c c} & |U\rangle & |L\rangle \\ \langle A| & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \langle B| & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{array}$$

    - Student B: I agree with you. Similarly, [BS2] acting on the lower state $|L\rangle$ causes a phase change of π in the path state $|C\rangle$ propagating toward detector D1 (multiplied by $e^{i\pi} = -1$). Thus, the matrix element $\langle C|BS1|L\rangle = -\frac{1}{\sqrt{2}}$. The remaining matrix elements are positive because the photon components do not undergo any phase shifts (see matrix [BS2] below).

$$[BS2] = \begin{array}{c|cc} & |U\rangle & |L\rangle \\ \langle C| & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \langle D| & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{array}$$

Do you agree with the students? Explain your reasoning.

B. Determining the matrix representation of the quantum mechanical operators that correspond to the mirrors (M)

Let's now consider the action of the **mirrors** on the photon states.

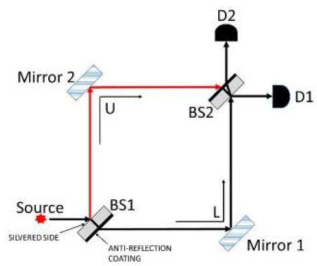


Figure 3

- In Figure 3, mirror 1 (M1) reflects only the photon state in the lower path and mirror 2 (M2) reflects only the photon state in the upper path. Thus, we can think of the mirrors as quantum mechanical reflection operators.
- The phase shifts of the photon state in the lower and upper paths due to reflection off the mirrors is π, and $e^{i\pi} = -1$. Both mirror operators are reflection operator that should multiply the incoming state by a factor $e^{i\pi} = -1$. Mirror 1 acts on the lower state and Mirror 2 acts on the upper state.
- We will denote the quantum mechanical operator corresponding to mirror 1 as [M1] and the quantum mechanical operator corresponding to mirror 2 as [M2].
- Since M1 only phase shifts the photon state in the lower path state $|L\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ by $e^{i\pi}$, [M1]=$\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$.
- Since M2 only phase shifts the photon state in the upper path state $|U\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ by $e^{i\pi}$, [M2]=$\begin{bmatrix}-1 & 0\\0 & 1\end{bmatrix}$.

10

14. Consider the following conversation between Student A and Student B:

- Student A: Suppose the initial state of the photon is the upper state, e.g., $|A\rangle = \begin{pmatrix}1\\0\end{pmatrix}$. After the photon propagates through BS1, the photon state is given by equation (1) which is
$$[\text{BS1}]\,|A\rangle = [\text{BS1}]\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\left[-\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix}$$
To check that the mirror operator [M1] only shifts the photon state in the lower path $|L\rangle = \begin{pmatrix}0\\1\end{pmatrix}$, we can write $\frac{1}{\sqrt{2}}[\text{M1}]\left[-\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\left[-\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\left[-\begin{pmatrix}1\\0\end{pmatrix}-\begin{pmatrix}0\\1\end{pmatrix}\right]$. So we see that $|L\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ has been phase shifted by π (multiplied by $e^{i\pi} = -1$).
- Student B: I agree. To check that the mirror operator [M2] only shifts the photon state in the upper path $|U\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, we can write
$\frac{1}{\sqrt{2}}[\text{M2}]\left[-\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{bmatrix}-1 & 0\\0 & 1\end{bmatrix}\left[-\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right]$. So we see that $|U\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ has been phase shifted by π (multiplied by $e^{i\pi} = -1$).

Do you agree with Student A and Student B's reasoning? Explain.

15. Mirror 1 and Mirror 2 produce reflection at the same time, e.g., $t = t_0$, on the photon state in the lower and upper paths, respectively. Therefore, the net effect of the mirrors on the state of the photon at time $t = t_0$ is the product of the two operators [M1][M2]. Combine the effects of the two mirrors on the photon state and find the matrix representation for the operator [M]=[M1][M2] that corresponds to the action of M1 and M2 on the photon state.

16. Consider the following conversation between two students:

- Student 1: The mirror operators corresponding to Mirror 1 and Mirror 2 operate on two different components of photon state, i.e., the upper path state and lower path state of the photon. Therefore, the mirror operators [M1] and [M2] commute. Thus, we can combine the mirror operators to find the net effect of the mirrors on the photon state, i.e., [M]=[M1][M2].
- Student 2: I agree with you. And since we chose our basis vectors to be in the order $|U\rangle$, $|L\rangle$, the matrix corresponding to the combined mirror operator is as follows:
$$[M] = \begin{array}{c|cc} & |U\rangle & |L\rangle \\ \hline \langle U| & -1 & 0 \\ \langle L| & 0 & -1 \end{array}$$
The diagonal matrix elements of [M] are -1 because the mirror operator causes a reflection of the photon state in the upper and lower paths, i.e., $\langle U|M|U\rangle = \langle U|-1|U\rangle = -1$ and $\langle L|M|L\rangle = \langle L|-1|L\rangle = -1$. The off-diagonal matrix elements are zero because of the orthogonality of the $|U\rangle$ and $|L\rangle$ path states, i.e, $\langle L|M|U\rangle = \langle L|-1|U\rangle = 0$ and $\langle U|M|L\rangle = \langle U|-1|L\rangle = 0$.
Do you agree with the students? Explain your reasoning.

C. Finding the action of the beam splitters and mirrors on an input state and their effect on the probability of a detector D1 or D2 "clicking" after a photon is emitted from the source

We now have the matrix representations of the beam splitters and mirrors:

[BS1]= $\frac{1}{\sqrt{2}}\begin{bmatrix}-1 & 1\\ 1 & 1\end{bmatrix}$

[BS2]= $\frac{1}{\sqrt{2}}\begin{bmatrix}1 & -1\\ 1 & 1\end{bmatrix}$

[M]= $\begin{bmatrix}-1 & 0\\ 0 & -1\end{bmatrix} = -1\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} = -\hat{I}$, where $\hat{I}$ is the identity operator.

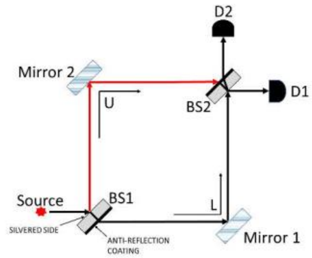


Figure 3

17. Find the action of these optical elements on a photon in an initial state $|A\rangle$ as shown in Figure 3 above, i.e., [BS2][M][BS1] $|A\rangle$.

18. Describe the implication of the answer to your preceding question on obtaining constructive or destructive interference at detectors D1 and D2 for the case in which the photons started in state $|A\rangle = \binom{1}{0}$.

19. In the MZI warm-up, you found that the phase shifts of the upper and lower paths were such that at detector D1 there was constructive interference and at detector D2 there was destructive interference for a photon that was initially in the state $|A\rangle = \begin{pmatrix}1\\0\end{pmatrix}$. Does your answer to question 18 agree with this earlier finding? Explain your reasoning.

20. Suppose the source is set up as in Figure 1.b such that the initial state of the photon is $|B\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. Find the action of [BS2][M][BS1]$|B\rangle$.

21. Consider the following conversation between two students:
    - Student 1: [BS2][M][BS1]=$\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$. So [BS2][M][BS1]$|A\rangle = \begin{pmatrix}1\\0\end{pmatrix}$. This implies that if the initial state of the photon is $|A\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, the photon will end up in detector D1 since that corresponds to the final path state $|C\rangle = \begin{pmatrix}1\\0\end{pmatrix}$.
    - Student 2. I agree with you. And [BS2][M][BS1]$|B\rangle = -\begin{pmatrix}0\\1\end{pmatrix}$, which implies that if the initial state of the photon is $|B\rangle = \begin{pmatrix}0\\1\end{pmatrix}$, the photon will end up in detector D2 since that corresponds to $|D\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. The expressions for the operators [BS1] and [BS2] we came up with were based upon how we defined the states corresponding to the A, B, U, L, C, and D paths.

    Do you agree with Student 1 and Student 2? Explain your reasoning.

22. Explain whether for the case in which the photons started in the state $|B\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ you will see constructive interference at detector D1 or D2.

❖ **Checkpoint**

- In figure 3, if the initial state of the photon is $|A\rangle = \begin{pmatrix}1\\0\end{pmatrix}$:
  - The final state of the photon is $\begin{pmatrix}1\\0\end{pmatrix}$.
  - The photon will always arrive at detector D1 since that corresponds to the final path state $|C\rangle = \begin{pmatrix}1\\0\end{pmatrix}$. There is completely constructive interference at detector D1.
  - The photon will never arrive at detector D2 because there is completely destructive interference at detector D2.
  - "Which-path" information is unknown.
- In figure 3, if the initial state of the photon is changed to $|B\rangle = \begin{pmatrix}0\\1\end{pmatrix}$:
  - The final state of the photon is $-\begin{pmatrix}0\\1\end{pmatrix}$.
  - The photon will always arrive in detector D2 since that corresponds to $|D\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. There is completely constructive interference at detector D1.
  - The photon will never arrive at detector D1 because there is completely destructive interference at detector D1.
  - "Which-path" information is unknown.

D. Determine the matrix representation of a quantum mechanical operator that corresponds to a phase shifter (PS) (e.g., a glass piece of a certain thickness inserted into one of the paths of the MZI)

Suppose we now insert a phase shifter (piece of glass with a certain thickness) in the upper path as shown in Figure 4 which shifts the photon state by a phase ϕ_{PS}.

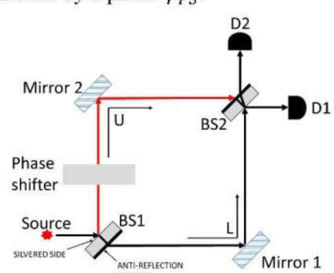


Figure 4

Let's find the matrix representation of the operator corresponding to the phase shifter.

- Recall that after the photon exits BS1, the photon state is
$$[\mathrm{BS1}]\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}-1 & 1\\ 1 & 1\end{bmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\left[-\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right]$$
- As shown in Figure 4, after the photon exits BS1, the next optical element to act on the photon state is the phase shifter (glass piece). Since the phase shifter is an operator which only acts on

the upper state because it is placed in the upper path, the matrix representation of the phase shifter $[PS_U]$ must shift the upper state like this: $\begin{pmatrix}1\\0\end{pmatrix} \rightarrow \begin{pmatrix}e^{i\phi_{PS}}\\0\end{pmatrix}$, but should not change the lower state $|L\rangle = \begin{pmatrix}0\\1\end{pmatrix}$.

- The only matrix that will accomplish this operation is $[PS_U]=\begin{bmatrix}e^{i\phi_{PS}} & 0\\0 & 1\end{bmatrix}$.

Let's check that the phase shifter operator only shifts the upper state $|U\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ by ϕ_{PS} and leaves the lower state $|L\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ unchanged, e.g,

$$[PS_U]\frac{1}{\sqrt{2}}\left[-\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{bmatrix}e^{i\phi_{PS}} & 0\\0 & 1\end{bmatrix}\left[-\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\left[-\begin{pmatrix}e^{i\phi_{PS}}\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right]$$

Note: φ_{PS} can be calculated if you are given the thickness of the phase shifter and the index of refraction, but in this homework φ_{PS} will be stated explicitly in each case.

23. What would be the matrix representation of the phase shifter if it was placed in the lower path (somewhere between BS1 and BS2) which shifts the photon state by a phase φ_{PS} in the lower path L?

24. Consider the following conversation between two students:
    - Student A: If we choose our basis vectors in the order $|U\rangle$, $|L\rangle$, the phase shifter which is placed in the upper path will have a matrix representation as shown below.

$$[PS_U] = \begin{array}{c|cc} & |U\rangle & |L\rangle \\ \langle U| & e^{i\phi_{PS}} & 0 \\ \langle L| & 0 & 1 \end{array}$$

    We can see this because the phase shifter in U path only affects the photon state along the upper path. The matrix elements can be found using the orthogonality conditions for the $|U\rangle$ and $|L\rangle$ path states, i.e., $\langle U|PS_U|U\rangle = \langle U|e^{i\phi_{PS}}|U\rangle = e^{i\phi_{PS}}$ and $\langle L|PS_U|U\rangle = \langle L|e^{i\phi_{PS}}|U\rangle = 0$.

    - Student B: I agree with you. Also, it makes sense that the operator corresponding to a phase shifter in the upper path does NOT affect the lower path state (it is equivalent to an identity operator in the lower path), so the matrix elements involving $|L\rangle$ are $\langle L|PS_U|L\rangle = \langle L|1|L\rangle = 1$ and $\langle U|PS_U|L\rangle = \langle U|1|L\rangle = 0$.

    Do you agree with the students? Explain your reasoning.

E. Finding probabilities of detectors "clicking" after a phase shifter is inserted due to intermediate interference at the detectors

For the following questions 25-29, assume Figure 4 is the setup of the MZI.

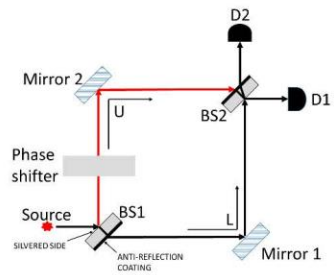


Figure 4

25. Let's suppose we know that the phase angle of the phase shifter is $\varphi_{PS} = \frac{7\pi}{5}$. What is the final state of the photon that starts in state $|A\rangle = \binom{1}{0}$ when it exits BS2? Hint: Use the matrix representations of the operators [BS1], [PS], [M], and [BS2] and act with these operators on the state $|A\rangle = \binom{1}{0}$ in the appropriate time-ordered manner.

26. Based upon your response to the preceding question, what is the probability that detector 1 clicks? (Hint: probability that detector D1 will click is $|\langle C|\Psi\rangle|^2$, where $|\Psi\rangle$ is the final state of the photon after it passes through BS2).

27. Based upon your response to question 25, what is the probability that detector 2 clicks? (Hint: probability that detector D2 will click is $|\langle D|\Psi\rangle|^2$, where $|\Psi\rangle$ is the final state of the photon after it passes through BS2).

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28. In the MZI warm-up, you found that inserting a phase shifter will create intermediate interference (neither completely constructive nor destructive) at both detectors with different probabilities. Do your answers to the preceding two questions agree with this? Explain your reasoning.

29. Consider the following conversation between two students about inserting a phase shifter into an MZI setup.
    - Student 1: The phase shifter can be used to check whether we have "which-path" information or not for a given MZI setup, but it does not cause interference (or a lack of interference). If we do not have "which-path" information for a particular MZI setup, interference is observed at the detectors. Inserting a phase shifter and gradually changing its phase shift <u>will</u> change the probabilities of the detectors registering a photon. However, if we have "which-path" information for a particular MZI setup, interference is not observed at the detectors and changing the phase shift of the phase shifter <u>will not</u> change the probabilities of the detectors registering a photon. In either case, inserting a phase shifter does not change whether or not interference is observed.
    - Student 2: I disagree with you. The phase shifter can cause a situation in which there is interference to change to a situation in which there is no interference. For example, before the phase shifter is inserted in the figure shown above, the probabilities of detector D1 and D2 registering a photon do not depend on the phase shift and thus we have "which-path" information. Once we insert the phase shifter, the probabilities of detectors D1 and D2 registering a photon <u>will</u> depend on the phase shift of the phase shifter. Thus, we do not have "which-path" information and no interference is observed.

With whom do you agree? Explain your reasoning.

❖ **Checkpoint**

- When a phase shifter is inserted into one of the paths of the MZI (see Figure 4):
  - There is intermediate interference at both detectors D1 and D2 with different probabilities.
  - The probability of a detector registering a photon depends on the phase angle of the phase shifter.
  - "Which-path" information is unknown.
  - The phase shifter can be used to check whether we have "which-path" information or not for a given MZI setup, but the insertion or removal of a phase shifter does not cause interference (or a lack of interference).

Removable BS2

- In the MZI tutorial, you learned that when BS2 is removed:
  - You have "which-path" information about the photon when the photon arrives at detectors D1 or D2 because the detectors D1 and D2 can only project one component of the photon path state.
  - In particular, detector D1 can only project the upper path state (state $|U\rangle = \binom{1}{0}$). Detector D2 can only project the lower path (state $|L\rangle = \binom{0}{1}$) (see Figure 5). There will no longer be interference observed at detectors D1 or D2 and the probability of each detector clicking is 50%, regardless of the relative phase difference of the two paths (because the photon will not interfere with itself if we have "which-path" information).

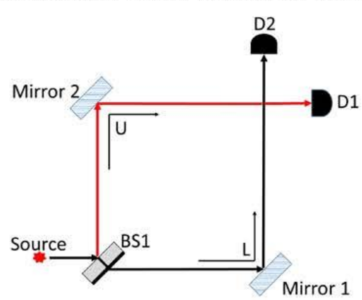

Figure 5

Let's check this mathematically. Suppose the photon state is initially $|A\rangle = \binom{1}{0}$.

The final state of the photon entering BS1 in state $|A\rangle = \binom{1}{0}$ after propagating through BS1 and reflecting off the mirrors is

$$[\mathrm{M}][\mathrm{BS1}]|A\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}\binom{1}{0} = \frac{1}{\sqrt{2}}\left[-\binom{1}{0} - \binom{0}{1}\right]$$

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30. Based upon the preceding discussion of the final state of the photon without BS2,

a) What is the probability that detector D1 will click for the case in Figure 5?

b) What is the probability that detector D2 will click for the case in Figure 5?

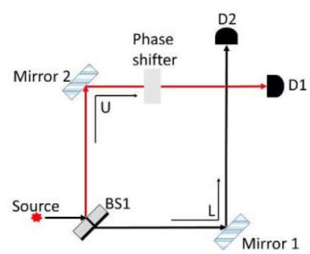

Figure 6

31. Suppose we now insert a glass piece in the upper path of the MZI, as shown in Figure 6.

(a) If the initial state of the photon is $|A\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, what is the final state of the photon before the state collapses due to interaction with the detectors D1 and D2?

(b) Based upon your response to the preceding question, what is the probability that detector D1 will click?

(c) Based on response to question 30 a), what is the probability that detector D2 will click?

(d) Does inserting a phase shifter (see Figure 6) into the U or L path of the MZI affect the probabilities of detectors D1 and D2 clicking for the case without BS2? (Hint: we have "which-path" information for the setup shown in figure 6.)

(e) Based upon your response to the preceding question, is there any interference observed at detectors D1 and D2 when BS2 is not present, as in Figure 6?

(f) Explain why there is no interference at detectors D1 and D2 without BS2.

❖ **Checkpoint**
- When BS2 is removed:
    - The probability of detector D1 and D2 registering a photon emitted from the source is 50% and does not depend on the phase angle of the phase shifter.
    - No interference is displayed at the detectors.
    - "Which-path" information is known.

32. A) Consider the following conversation between three students:

- Student A: The operators for BS1, BS2, mirrors, and phase shifter that we found are hermitian operators and correspond to physical observables.
- Student B: I disagree with you. The operators for BS1, BS2, mirrors, and phase shifter that we found are unitary operators and help us find how the state evolves in time at different instants.
- Student C: I think these operators (BS1, BS2, mirrors, and phase shifter) that we found are both hermitian and unitary.

Explain why you agree or disagree with each student.

29. B) If an operator U is hermitian, then $U = U^\dagger = (U^T)^*$. Which of the operators (BS1, BS2, mirror, and phase shifter) are hermitian operators? Do these operators correspond to physical observables (a property that can be measured, e.g., position, momentum, or energy)? If an operator corresponds to a physical observable, must that operator be hermitian?

29. C) If an operator U is unitary, then $U^\dagger U = \hat{I}$, where $\hat{I}$ is the identity operator. Unitary operators preserve the norm, or inner product, of the physical space. All time evolution operators must be unitary operators. Which of the operators (BS1, BS2, mirror, and phase shifter) are unitary operators?

❖ **Checkpoint**

- The operators for BS1, BS2, mirrors, and phase shifter <u>are not Hermitian</u> operators because they do not correspond to physical observables. If one of the operators satisfies the equality $U = U^\dagger = (U^T)^*$, it is a coincidence.
- The operators for BS1, BS2, mirrors, and phase shifter <u>are unitary</u> because they are time evolution operators which preserve the norm, or inner product of the physical space.

A.2 HYBRID QuILT SECTION WITH POLARIZERS

Understanding the Mach-Zehnder Interferometer (MZI) with Single Photons: Homework 2

The goals of this homework are to use a simplified ideal version of MZI to help you:

- **Connect qualitative understanding of the MZI with a simple mathematical model by**
  - A. **Determining the product space of path states and polarization states for a polarized photon in the U and L paths**
  - B. **Determining the matrix representation in a given basis of the quantum mechanical operators that correspond to beam splitter 1, beam splitter 2, mirrors, phase shifter, and polarizers**
  - C. **Finding the effect of various quantum mechanical "time-evolution" operators on an input state and the probability of detector D1 or D2 clicking for four cases:**
    - i. **Original MZI setup with a phase shifter in the upper path**
    - ii. **Horizontal polarizer in upper path, phase shifter in upper path, and vertical polarizer in lower path**
    - iii. **Horizontal polarizer in upper path, phase shifter in upper path, vertical polarizer in lower path, and 45 degree polarizer placed in the lower path between BS2 and detector D1**
    - iv. **Horizontal polarizer and phase shifter in upper path**

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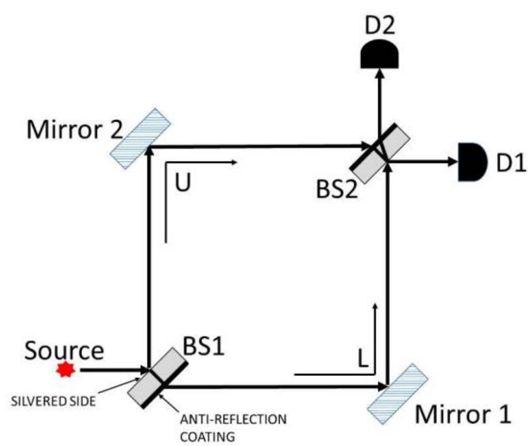
The setup for the ideal Mach-Zehnder Interferometer (MZI) shown below is as follows:

- The photons originate from a monochromatic coherent point source. (Note: Experimentally, a source can only emit nearly monochromatic photons such that there is a very small range of wavelengths coming from the source. Here, we assume that the photons have negligible "spread" in energy.)
- Assume that the photons propagating through both the U and L paths travel the same distance in vacuum to reach each detector.
- All angles of incidence are 45° with respect to the normal to the surface.
- For simplicity, we will assume that a photon can only reflect from one of the two surfaces of the identical half-silvered mirrors (beam splitters) BS1 and BS2 because of an anti-reflection coating on one of the surfaces.
- Assume that beam splitters BS1 and BS2 are infinitesimally thin so that there is no phase shift when a photon propagates through them.
- The phase shifter is ideal and non-reflective.
- Ignore the effect of polarization of the photons due to reflection by the beam splitters or mirrors.
- The photo-detectors D1 and D2 are point detectors located symmetrically with respect to the other components of the MZI as shown.
- All photo-detectors are ideal and 100% efficient.
- Polarizers do not introduce phase shifts.
- All measurements are ideal projective measurements.
- "Which-path" information is known when each detector D1 and D2 shown below can only project the component of the photon state along the U path or the L path. "Which-path" information is unknown when each detector D1 and D2 can project both the U and L components of the photon state.
- For the entire tutorial, assume that a large number of photons (N) are sent one at a time.



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Before we begin, we will make a few assumptions and observations:

- In all of the matrix representations of the operators, in a given basis, we will simplify the "≐" sign which means "is represented in a given basis by" with "=" for convenience.
- The beam splitters are 50/50 splitters, meaning that a measurement of the photon position immediately after it exits the beam splitter BS1 would yield an outcome such that the photon is either in the upper path or the lower path with 50% probability.
- The silvered side of the beam splitter is the point of reflection. No reflection occurs at the air-glass interface (the bold side of the beam splitter), due to anti-reflection coatings.
- From here on, assume that the thickness of the beam splitters is negligible so the phase shift introduced by the propagation of light through the beam splitters is zero ($\varphi_{BS} = 0$).
- No relative phase shift is introduced when a photon propagates through vacuum because the photon travels the same distance in vacuum along each of the U and L paths.
- The upper path U is marked in RED. The lower path L is marked in BLACK.
- $|U\rangle$ is the photon state corresponding to the U path and $|L\rangle$ is the photon state corresponding to the L path. $|V\rangle$ is the photon polarization state corresponding to vertical polarization and $|H\rangle$ is the photon polarization state corresponding to horizontal polarization.
- When determining the matrix operators in the two dimensional Hilbert space for the photon path states, assume the basis vectors are taken in the order $|U\rangle$, $|L\rangle$.
- When determining the matrix operators in the two dimensional Hilbert space for the photon polarization states, assume the basis vectors are taken in the order $|V\rangle$, $|H\rangle$.
- When determining the matrix operators in the four dimensional product space involving both the photon path states and polarization states, assume the basis vectors are taken in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$.
- As shown in Figure 2, we will denote the photon path states entering BS1 as $|U\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and $|L\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. We will denote photon state propagating towards detector D1 as path state $|U\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and the photon state propagating towards detector D2 as the path state $|L\rangle = \begin{pmatrix}0\\1\end{pmatrix}$.

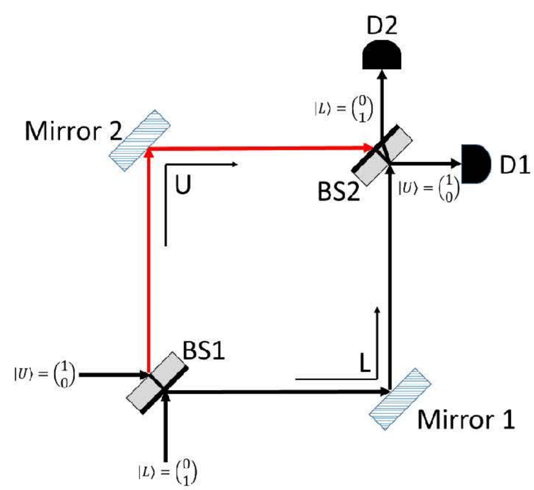

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Figure 2

Table 1: Phase shifts of a photon state due to reflection, transmission, and propagation through a medium

	Initially in medium with lower *n*	Initially in medium with higher *n*
Reflection at interface	Phase shift of π	No phase shift
Transmission at interface	No phase shift	No phase shift
Propagation through a medium	Phase shift φ depends on thickness and refractive index *n* of the medium	

A. Determine the product space for a polarized photon in the U and L paths

- You have already learned that the photon states corresponding to the U and L paths can be represented as two linearly independent states, such as $|U\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and $|L\rangle = \begin{pmatrix}0\\1\end{pmatrix}$, since the Hilbert space is two dimensional. The $|U\rangle$ and $|L\rangle$ states are orthogonal, e.g., $\langle U|L\rangle = \langle L|U\rangle = 0$ and normalized, e.g., $\langle U|U\rangle = \langle L|L\rangle = 1$.
- Any operator in a two dimensional Hilbert space can be represented by a 2×2 matrix in the chosen basis.
- When polarizers are added, we must consider the Hilbert space corresponding to the polarization state of the photon.
- The Hilbert space involving both path states (from the U and L paths) and polarization states is a product space.
- Let's choose a basis in which we denote the polarization state of the vertically polarized photon to be $|V\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and the polarization state of the horizontally polarized photon to be $|H\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. These two polarizations are linearly independent and all other photon polarizations can be constructed from these states, e.g., $|{+45°}\rangle = \frac{1}{\sqrt{2}}(|V\rangle + |H\rangle)$. The Hilbert space for the polarization of the photon is also two dimensional (similar to the Hilbert space for the path states). The $|V\rangle$ and $|H\rangle$ polarization states are orthogonal, e.g., $\langle V|H\rangle = \langle H|V\rangle = 0$ and normalized, e.g., $\langle V|V\rangle = 1$ and $\langle H|H\rangle = 1$.
- The product space of the polarization states $|V\rangle$ and $|H\rangle$ and the path states $|U\rangle$ and $|L\rangle$ is four dimensional. There are four possible basis states in the product space: $|U\rangle|V\rangle$, $|U\rangle|H\rangle$, $|L\rangle|V\rangle$, and $|L\rangle|H\rangle$.
- To determine the matrix representation for the photon states $|U\rangle|V\rangle$, $|U\rangle|H\rangle$, $|L\rangle|V\rangle$, and $|L\rangle|H\rangle$, we find the basis states in the product space (tensor product of path states and polarization states which takes us from two dimensional Hilbert spaces to a four dimensional Hilbert space):
  - $|U\rangle \otimes |V\rangle = |U\rangle|V\rangle = |UV\rangle$
  - $|U\rangle \otimes |H\rangle = |U\rangle|H\rangle = |UH\rangle$
  - $|L\rangle \otimes |V\rangle = |L\rangle|V\rangle = |LV\rangle$
  - $|L\rangle \otimes |H\rangle = |L\rangle|H\rangle = |LH\rangle$
- Let's define a tensor product of two general two-dimensional vectors $|a\rangle$ and $|b\rangle$ as

$$|a\rangle \otimes |b\rangle = \begin{pmatrix}a_1\\a_2\end{pmatrix} \otimes \begin{pmatrix}b_1\\b_2\end{pmatrix} = \begin{pmatrix}a_1b_1\\a_1b_2\\a_2b_1\\a_2b_2\end{pmatrix}$$

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1. Keeping this in mind, find the matrix representation for the four possible photon states $|U\rangle|V\rangle = |UV\rangle$, $|U\rangle|H\rangle = |UH\rangle$, $|L\rangle|V\rangle = |LV\rangle$, and $|L\rangle|H\rangle = |LH\rangle$ using $|U\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, $|L\rangle = \begin{pmatrix}0\\1\end{pmatrix}$, $|V\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, and $|H\rangle = \begin{pmatrix}0\\1\end{pmatrix}$.

2. Consider the following conversation between two students about a +45° polarized photon emitted from the source shown in Figure 1. Assume that the +45° means that the polarization is rotated 45° counterclockwise from the horizontal, like this:

- Student 1: If the photon is emitted from the source in the path state $|U\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ (as shown in Figure 1) with +45° polarization, then the initial photon state can be denoted like this:

$$|U\rangle \otimes |45°\rangle = |U, +45°\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix}\right] = \begin{pmatrix}1\\0\end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\\0\\0\end{pmatrix}.$$

- Student 2: I disagree with you. The final state, $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\\0\\0\end{pmatrix}$, you found corresponds to a source emitting a photon with -45° polarization. Actually, the state of a +45° polarized photon in the upper path should look like this:

$$|U\rangle|45°\rangle = |U\rangle \otimes |45°\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\right] = \begin{pmatrix}1\\0\end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix}.$$

With whom do you agree? Explain your reasoning.

B. Determine the matrix representations of the quantum mechanical operators that correspond to beam splitter 1, beam splitter 2, mirrors, phase shifter, and polarizers

i. **Determining the matrix representations of beam splitters 1 and 2**

- Previously, you found that the matrix representations for the quantum mechanical operators corresponding to beam splitter 1 and beam splitter 2 in the two dimensional Hilbert space (only taking into account the photon path states) are

$$[\text{BS1}]=\frac{1}{\sqrt{2}}\begin{bmatrix}-1 & 1\\ 1 & 1\end{bmatrix}$$

$$[\text{BS2}]=\frac{1}{\sqrt{2}}\begin{bmatrix}1 & -1\\ 1 & 1\end{bmatrix}$$

assuming the basis vectors are taken in the order $|U\rangle$, $|L\rangle$.

- Now we need to determine what these operators look like in the four dimensional product space (taking into account both the photon <u>path states</u> and <u>polarization states</u>).
- Beam splitter 1 and beam splitter 2 only affect the path states $|U\rangle$ and $|L\rangle$, NOT the polarization states $|H\rangle$ and $|V\rangle$ of the photon.
- We will always use the following convention for the order of the basis vectors when determining all the 4×4 matrices corresponding to the optical elements (BS1, BS2, mirrors, phase shifter, and polarizers) in the product space: $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$.
- Predict the various matrix elements corresponding to beam splitter 1 below in the boxes (Hints are provided below to find these matrix elements).

$$[BS1] = \begin{array}{c|cccc} & |UV\rangle & |UH\rangle & |LV\rangle & |LH\rangle \\ \langle UV| & \square & \square & \square & \square \\ \langle UH| & \square & \square & \square & \square \\ \langle LV| & \square & \square & \square & \square \\ \langle LH| & \square & \square & \square & \square \end{array}$$

- In homework 1, you learned that BS1 reflects the photon path state by π, so there is a phase shift of the upper path state by $e^{i\pi} = -1$. The lower path state is not phase shifted. Thus, $[BS1]|U\rangle = \frac{1}{\sqrt{2}}(-|U\rangle + |L\rangle)$.
- The beam splitters do not affect the polarization state of the photon, i.e., $[BS1]|UV\rangle = \frac{1}{\sqrt{2}}(-|UV\rangle + |LV\rangle)$ and $[BS1]|UH\rangle = \frac{1}{\sqrt{2}}(-|UH\rangle + |LH\rangle)$.
- Therefore, the matrix elements $\langle UV|BS1|UV\rangle$ and $\langle UH|BS1|UH\rangle$ are $\langle UV|BS1|UV\rangle = \langle UV|\frac{1}{\sqrt{2}}(-|UV\rangle + |LV\rangle) = -\frac{1}{\sqrt{2}}$ and $\langle UH|BS1|UH\rangle = \langle UH|\frac{1}{\sqrt{2}}(-|UH\rangle + |LH\rangle) = -\frac{1}{\sqrt{2}}$.
- The matrix elements $\langle UV|BS1|UH\rangle = 0$ and $\langle UH|BS1|UV\rangle = 0$ (because of the orthogonality of $|V\rangle$ and $|H\rangle$, e.g., $\langle V|H\rangle = 0$ and $\langle H|V\rangle = 0$ in the polarization state subspace). (Note that the operator [BS1] does not affect the polarization state of the photon.) So the matrix elements that mix different polarizations, $\langle UV|BS1|UH\rangle$ and $\langle UH|BS1|UV\rangle$, are $\langle UV|BS1|UH\rangle = \langle UV|\frac{1}{\sqrt{2}}(-|UH\rangle + |LH\rangle) = 0$ and $\langle UH|BS1|UV\rangle = \langle UH|\frac{1}{\sqrt{2}}(-|UV\rangle + |LV\rangle) = 0$.
- Thus, we can fill in the upper quadrant like this:

$$[BS1] = \begin{array}{c|cccc} & |UV\rangle & |UH\rangle & |LV\rangle & |LH\rangle \\ \langle UV| & -\frac{1}{\sqrt{2}} & 0 & \square & \square \\ \langle UH| & 0 & -\frac{1}{\sqrt{2}} & \square & \square \\ \langle LV| & \square & \square & \square & \square \\ \langle LH| & \square & \square & \square & \square \end{array}$$

3. Keeping in mind the phase shifts for the photon path states $|U\rangle$ and $|L\rangle$ in the setup given in Figure 1 and the orthogonality conditions of the path states $|U\rangle$ and $|L\rangle$ and polarization states $|H\rangle$ and $|V\rangle$, fill in the rest of the matrix for operator [BS1] shown above in the product space of path states and polarization states.

- The matrix representation of beam splitter 1 that you should have determined in the previous question is

$$[BS1] = \frac{1}{\sqrt{2}}\begin{bmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

If this does not match your answer to the previous question, go back and check your work.

4. Consider the following conversation between two students about the [BS1] matrix using the basis vectors in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$.
- Student 1: When I calculated the matrix elements of [BS1], I obtained $[BS1] = \frac{1}{\sqrt{2}}\begin{bmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$. This makes sense because there is $e^{i\pi} = -1$ along the diagonal in the $|UV\rangle$, $|UH\rangle$ subspace (or upper left quadrant), which means that the component of the photon state in the upper path has been phase shifted by π.
- Student 2: I agree with you. And in the other quadrants, there are 1's along the diagonal. This means that [BS1] does not lead to any phase change in those subspaces. In particular, [BS1] does not change the phase of the photon state in the $|LV\rangle$, $|LH\rangle$ subspace. Actually, we can observe a relationship between the [BS1] matrix in the 2×2 space involving only the photon path states and the [BS1] matrix in the 4×4 product space involving both photon path states and polarization states as follows:

$$[BS1] = \frac{1}{\sqrt{2}}\begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \rightarrow [BS1] = \frac{1}{\sqrt{2}}\begin{bmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}.$$

Do you agree with the students? Explain your reasoning.

- Now we need to find the matrix representation for the operator corresponding to beam splitter 2. Predict the matrix corresponding to the operator for beam splitter 2 in Figure 1 which does not affect polarization. (Hints will be provided below to answer this question.)

5. Keeping in mind the phase shifts from Table 1, determine the action of [BS2] on the upper and lower path states:

(a) $[BS2]|UV\rangle =$ ________________________________

(b) $[BS2]|UH\rangle =$ ________________________________

(c) $[BS2]|LV\rangle =$ ________________________________

(d) $[BS2]|LH\rangle =$ ________________________________

6. Using the orthogonality conditions $\langle U|L\rangle = \langle L|U\rangle = 0$ and $\langle V|H\rangle = \langle H|V\rangle = 0$ for the corresponding two-dimensional subspace, fill in the matrix for [BS2].

$$[BS2] = \begin{array}{c|cccc} & |UV\rangle & |UH\rangle & |LV\rangle & |LH\rangle \\ \hline \langle UV| & \square & \square & \square & \square \\ \langle UH| & \square & \square & \square & \square \\ \langle LV| & \square & \square & \square & \square \\ \langle LH| & \square & \square & \square & \square \end{array}$$

- The matrix representation of [BS2] that you should have determined in the previous question is

$$[BS2] = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

If this does not match your answer to the previous question, go back and check your work.

ii. Determining the matrix representations corresponding to the mirrors

- Earlier, when you only considered photon path states, you found the matrix corresponding to both of the mirrors in Figure 1 as $[M] = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} = -1\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = -\hat{I}$, where $\hat{I}$ is the identity operator.

7. The mirror operator in a particular path only changes the path state of the photon by $e^{i\pi} = -1$. It does not affect the polarization state. Keeping this in mind, write down the matrix corresponding to both of the mirror operators for the product space involving both the photon path state and photon polarization state. Assume the basis vectors are taken in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$.

$$[M] = \begin{bmatrix} \square & \square & \square & \square \\ \square & \square & \square & \square \\ \square & \square & \square & \square \\ \square & \square & \square & \square \end{bmatrix}$$

iii. **Determining the matrix representations corresponding to a phase shifter, e.g., a piece of glass placed in the upper or lower path**

- Earlier, when you only considered photon path states, you found the matrix corresponding to a phase shifter operator in the upper path as $[PS_U] = \begin{bmatrix} e^{i\phi_{PS}} & 0 \\ 0 & 1 \end{bmatrix}$.

8. The phase shifter in a particular path only changes the path state of the photon by $e^{i\varphi_{PS}}$, in which φ_{PS} is the phase shift due to the phase shifter. The phase shifter does not affect the polarization state of the photon. Keeping this in mind, write down the matrix corresponding to the phase shifter operator for a phase shifter placed anywhere in the upper path between BS1 and BS2. Assume the basis vectors are taken in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$.

$$[PS_U] = \begin{bmatrix} \square & \square & \square & \square \\ \square & \square & \square & \square \\ \square & \square & \square & \square \\ \square & \square & \square & \square \end{bmatrix}$$

9. Write down the matrix corresponding to the phase shifter operator for a phase shifter placed in the lower path between BS1 and BS2.

$$[PS_L] = \begin{bmatrix} \square & \square & \square & \square \\ \square & \square & \square & \square \\ \square & \square & \square & \square \\ \square & \square & \square & \square \end{bmatrix}$$

10. Consider the following conversation between two students about the representation of the phase shifter operators, $[PS_U]$ and $[PS_L]$, assuming the basis vectors are taken in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$.
    - Student A: Placing a phase shifter in the upper path only affects the phase of the component of the photon state in the upper path. So it makes sense that the operator $[PS_U] = \begin{bmatrix} e^{i\varphi_{ps}} & 0 & 0 & 0 \\ 0 & e^{i\varphi_{ps}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$, since in the $|UV\rangle$, $|UH\rangle$ subspace we have the matrix element $e^{i\varphi_{PS}}$ along the diagonal. We see 1's along the diagonal in the $|LV\rangle$, $|LH\rangle$ subspace because the phase shifter does not act on the component of the photon state in the lower path, so in that subspace we have an identity operator.
    - Student B: I agree with you. And a phase shifter operator in the lower path looks like $[PS_L] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{i\varphi_{ps}} & 0 \\ 0 & 0 & 0 & e^{i\varphi_{ps}} \end{bmatrix}$ because the phase shifter only acts on the component of the photon state in the

lower path. We have the matrix elements $e^{i\varphi_{PS}}$ along the diagonal in the $|LV\rangle$, $|LH\rangle$ subspace. And we have 1's along the diagonal in the $|UV\rangle$, $|UH\rangle$ subspace (an identity operator) because the phase shifter does not act on the component of the photon state in the upper path. We can observe a relationship between the phase shifter matrix in the 2×2 space involving only the photon path states and the phase shifter matrix in the 4×4 product space involving both the photon path states and polarization states as follows:

$$[PS_U] = \begin{bmatrix} e^{i\phi_{PS}} & 0 \\ 0 & 1 \end{bmatrix} \rightarrow [PS_U] = \begin{bmatrix} e^{i\varphi_{ps}} & 0 & 0 & 0 \\ 0 & e^{i\varphi_{ps}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Do you agree with the students? Explain your reasoning.

- In summary, the matrices corresponding to the mirror operator and phase shifter operators in the upper or lower path in the product space that includes path and polarization states are
  - $[M] = -\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = -\hat{I}$, where $\hat{I}$ is the identity operator.
  - $[PS_U] = \begin{bmatrix} e^{i\varphi_{ps}} & 0 & 0 & 0 \\ 0 & e^{i\varphi_{ps}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$, where φ_{PS} is the phase shift due to the phase shifter.
  - $[PS_L] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{i\varphi_{ps}} & 0 \\ 0 & 0 & 0 & e^{i\varphi_{ps}} \end{bmatrix}$, where φ_{PS} is the phase shift due to the phase shifter.

  If these matrices do not match your answers to the previous questions, go back and check your work.

iv. Determining the matrix representations of the operators corresponding to polarizers

- Let's first recapitulate how a polarizer acts on the photon polarization states $|V\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|H\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ in a <u>two dimensional space</u> before we consider the product space which also includes the photon path states $|U\rangle$ and $|L\rangle$.
- We will define the matrix representing a vertical polarizer as $[P_V]$ and the matrix representing a horizontal polarizer as $[P_H]$ and we will use the following convention for the matrix representation of polarizer operators in the two dimensional Hilbert space (i.e., choose the states in the order $|V\rangle$, $|H\rangle$ to write the matrix elements of $[P_V]$ and $[P_H]$):

$$\begin{array}{c|cc} & |V\rangle & |H\rangle \\ \hline \langle V| & \square & \square \\ \langle H| & \square & \square \end{array}$$

- A vertical polarizer will allow a vertically polarized photon to pass through and will completely block a horizontally polarized photon. So we know that $[P_V]|V\rangle = [P_V]\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix}$ and $[P_V]|H\rangle = [P_V]\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix}$.

11. Consider the following statement from Student 1:
    - Student 1: The matrix corresponding to the vertical polarizer operator is $[P_V] = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}$, since the matrix elements are

      $\langle V|P_V|V\rangle = (1\quad 0)[V]\begin{pmatrix}1\\0\end{pmatrix} = (1\quad 0)\begin{pmatrix}1\\0\end{pmatrix} = 1$

      $\langle H|P_V|V\rangle = (0\quad 1)[V]\begin{pmatrix}1\\0\end{pmatrix} = (0\quad 1)\begin{pmatrix}1\\0\end{pmatrix} = 0$

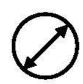
      $\langle V|P_V|H\rangle = (1\quad 0)[V]\begin{pmatrix}0\\1\end{pmatrix} = (1\quad 0)\begin{pmatrix}0\\0\end{pmatrix} = 0$

      $\langle H|P_V|H\rangle = (0\quad 1)[V]\begin{pmatrix}0\\1\end{pmatrix} = (0\quad 1)\begin{pmatrix}0\\0\end{pmatrix} = 0$

Do you agree with Student 1? Explain your reasoning.

12. In the preceding question, Student 1's reasoning is correct for finding the matrix elements for the vertical polarizer operator in the given basis. Using the information above, write down the matrix corresponding to the <u>horizontal</u> polarizer operator $[P_H]$ for the two dimensional polarization Hilbert space assuming that the basis vectors are chosen in the order $|V\rangle$, $|H\rangle$.

- Now you will determine the matrix corresponding to a +45° polarizer operator, $[P_{+45°}]$. Assume that the +45° polarizer operator has a polarization axis which has been rotated counterclockwise 45° from the horizontal, like this:



  The normalized state of a +45° polarized photon can be written as an equal superposition of the states $|V\rangle$ and $|H\rangle$ as follows:

  $|45°\rangle = \frac{1}{\sqrt{2}}(|V\rangle + |H\rangle) = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$.
- The state of a -45° polarized photon can be written as

  $|-45°\rangle = \frac{1}{\sqrt{2}}(-|V\rangle + |H\rangle) = \frac{1}{\sqrt{2}}\left[-\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix}$.
- A +45° polarizer, $[P_{+45°}]$, will allow a +45° polarized photon to pass through and will completely block a -45° polarized photon. So $[P_{+45°}]\,|45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ and $[P_{+45°}]\,|-45°\rangle = \begin{pmatrix}0\\0\end{pmatrix}$.

13. Which one of the following matrices represents the +45° polarizer operator, $[P_{+45°}]$, if the basis vectors are chosen in the order $|V\rangle$, $|H\rangle$?

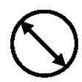
    (a) $[P_{+45°}] = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$

    (b) $[P_{+45°}] = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

    (c) $[P_{+45°}] = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

    (d) $[P_{+45°}] = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$

14. Which one of the following matrices represents the -45° polarizer operator, $[P_{-45°}]$, if the basis vectors are chosen in the order $|V\rangle$, $|H\rangle$? Note: the -45° polarizer operator has been rotated 45° clockwise from the horizontal, like this:



    (a) $[P_{-45°}] = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$

    (b) $[P_{-45°}] = \frac{1}{2}\begin{bmatrix} -1 & -1 \\ -1 & 1 \end{bmatrix}$

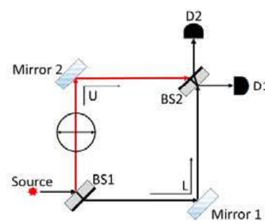
    (c) $[P_{-45°}] = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

    (d) $[P_{-45°}] = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$

- In summary, if the basis vectors are chosen in the order $|V\rangle$, $|H\rangle$, then
    - The matrix corresponding to the vertical polarizer is $[P_V] = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$.
    - The matrix corresponding to the horizontal polarizer is $[P_H] = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$.
    - The matrix corresponding to the +45° polarizer is $[P_{+45°}] = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$.
    - The matrix corresponding to the -45° polarizer is $[P_{-45°}] = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$.

  If your answers to the preceding questions do not match these, go back and check your work.

- Now you will find the matrices corresponding to the vertical, horizontal, and +45° polarizer operators in the four dimensional product space by including both photon polarization and path states.
- Suppose we change the original MZI setup by placing a horizontal polarizer in the upper path, as follows:



- The horizontal polarizer in the upper path will only affect the component of the photon state in the upper path. It will block the vertical polarization component of the photon state in the upper path and will let the horizontal polarization component of the photon state in the upper path pass through. It will not affect the component of the photon state in the lower path.
- We will always use the following convention for the order in which the basis vectors are chosen to determine the matrices for the polarizer operators in the product space: $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$.

15. Consider the following conversation between students about the matrix corresponding to a horizontal polarizer operator in the upper path, $[P_{UH}]$, for the setup shown in the figure above (basis vectors are chosen in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$):
    - Student 1: The matrix corresponding to a horizontal polarizer operator in the upper path is $[P_{UH}] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$, since the only matrix element that survives is $\langle UH|P_{UH}|UH\rangle = 1$. We can see that $\langle LH|P_{UH}|LH\rangle = 0$ and $\langle LV|P_{UH}|LV\rangle = 0$ because the operator $[P_{UH}]$ acting on the L path state must be zero.
    - Student 2: I disagree with you. The matrix corresponding to a horizontal polarizer in the upper path should look like $[P_{UH}] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$ because $\langle LH|P_{UH}|LH\rangle = 1$ and $\langle LV|P_{UH}|LV\rangle = 1$. The operator $[P_{UH}]$ acting on the L path state of the photon must not change the L path state, so $[P_{UH}]$ returns the same state back, as follows: $\langle LH|P_{UH}|LH\rangle = \langle LH|LH\rangle = 1$ and $\langle LV|P_{UH}|LV\rangle = \langle LV|LV\rangle = 1$. $[P_{UH}]$ is an identity operator in the L path subspace (lower right quadrant) of the full 4×4 matrix for the setup shown above.

- Student 3: I think the matrix corresponding to a horizontal polarizer in the upper path should look like $[P_{UH}] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$, since the horizontal polarizer only allows the horizontally polarized photons to pass through.

With whom do you agree? Explain your reasoning.

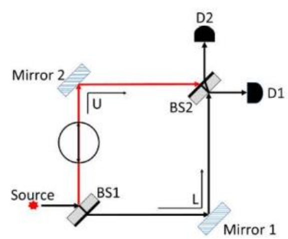
If you did not agree with Student 2 in the preceding question, go back and check your work.

16. Which one of the following matrices represents the <u>horizontal polarizer operator in the lower path, $[P_{LH}]$</u>, if the basis vectors are chosen in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$?

(a) $[P_{LH}] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$ (c) $[P_{LH}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

(b) $[P_{LH}] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$ (d) $[P_{LH}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

- Suppose we place a vertical polarizer in the upper path of the MZI, like this:



- The vertical polarizer in the upper path will only affect the component of the photon state in the upper path. It will block the horizontal polarization component of the photon state in the upper path and will let the vertical polarization component of the photon state in the upper path pass through.

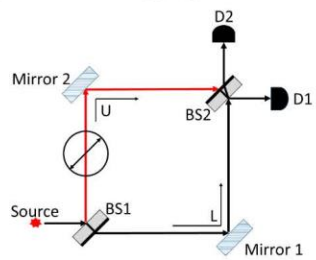
17. Which one of the following matrices represents the <u>vertical polarizer operator in the upper path, $[P_{UV}]$</u>, (shown above) if the basis vectors are chosen in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$?

(a) $[P_{UV}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$ (c) $[P_{UV}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$

(b) $[P_{UV}] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$ (d) $[P_{UV}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

18. Write down the matrix corresponding to a vertical polarizer operator in the lower path, $[P_{LV}]$, given that the answer to the previous question is (d).

- Suppose we place a +45° polarizer in the upper path, like this:



- In the two dimensional space, you already determined that the matrix corresponding to the +45° polarizer operator is $[P_{+45°}] = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ in the $|V\rangle$, $|H\rangle$ basis.
- The +45° polarizer in the upper path will affect the component of the polarization state of a photon in the upper path and will not affect the component of the polarization state of a photon in the lower path.

19. Choose the matrix which represents the +45° polarizer operator in the upper path, $[P_{U_{+45°}}]$, assuming that the basis vectors are chosen in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$.
Hint: When you act with the +45° polarizer operator, $[P_{U_{+45°}}]$, on a photon in the upper path with +45° polarization, i.e., $|U\rangle|45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}$, it should allow the photon to pass through without any change, as follows:

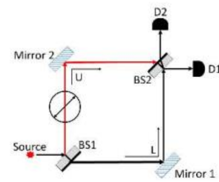
$[P_{U_{+45°}}]|U\rangle|45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}$. On the other hand, $[P_{U_{+45°}}]$ should block a photon in the upper path with -45° polarization, i.e., $[P_{U_{+45°}}]|U\rangle|-45°\rangle = [P_{+45°_U}]\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$.

(a) $[P_{U_{+45°}}] = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

(b) $[P_{U_{+45°}}] = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$

(c) $\left[P_{U_{+45^\circ}}\right] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$ (d) $\left[P_{U_{+45^\circ}}\right] = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

20. Consider the following conversation between two students about the answer to the preceding questions:

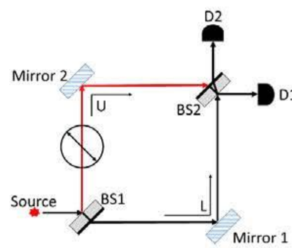


- Student A: I believe that the matrix corresponding to the +45° polarizer operator $[P_{U_{+45^\circ}}]$ in the upper path, as shown in the figure above, should look like $\left[P_{U_{+45^\circ}}\right] = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$. The +45° polarizer operator only changes the photon state in the subspace of the U path state.
- Student B: I agree with you. And in the subspace of the L path state (lower right quadrant), the +45° polarizer operator in the upper path, $\left[P_{U_{+45^\circ}}\right]$, acts as an identity operator because it does not change the component of the photon state in the L path.

Do you agree with the students? Explain your reasoning.

21. Now write down the matrix corresponding to a +45° polarizer operator in the lower path, $\left[P_{L_{+45^\circ}}\right]$, if basis vectors are chosen in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$.

- Suppose we place a -45° polarizer in the upper path, as follows:



22. Choose the matrix which represents the -45° polarizer operator in the upper path, $[P_{U_{-45°}}]$, assuming that the basis vectors are chosen in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$.
Hint: When you act with the -45° polarizer operator in the upper path on the photon state in the upper path with -45° polarization, i.e., $|U\rangle|-45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\\0\\0\end{pmatrix}$, it should allow the photon to pass through without any change, as follows:
$[P_{U_{-45°}}]|U\rangle|-45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\\0\\0\end{pmatrix}$. On the other hand, it should block a photon in the upper path with +45° polarization, i.e., $[P_{U_{-45°}}]|U\rangle|+45°\rangle = [P_{U_{-45°}}]\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix} = \begin{pmatrix}0\\0\\0\\0\end{pmatrix}$.

(a) $[P_{U_{-45°}}] = \begin{bmatrix}\frac{1}{2} & -\frac{1}{2} & 0 & 0\\ -\frac{1}{2} & \frac{1}{2} & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}$

(b) $[P_{U_{-45°}}] = \begin{bmatrix}-\frac{1}{2} & \frac{1}{2} & 0 & 0\\ \frac{1}{2} & -\frac{1}{2} & 0 & 0\\ 0 & 0 & 1 & 1\\ 0 & 0 & 1 & 1\end{bmatrix}$

(c) $[P_{U_{-45°}}] = \begin{bmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0\\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0\\ 0 & 0 & 1 & 1\\ 0 & 0 & 1 & 1\end{bmatrix}$

(d) $[P_{U_{-45°}}] = \begin{bmatrix}1 & 1 & 0 & 0\\ 1 & 1 & 0 & 0\\ 0 & 0 & 1 & 1\\ 0 & 0 & 1 & 1\end{bmatrix}$

23. Write down the matrix corresponding to a -45° polarizer operator in the lower path, $[P_{L_{-45°}}]$, if basis vectors are chosen in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, $|LH\rangle$.

24. Consider the following conversation between students:
   - Student 1: I believe the polarizer operators we have found are both hermitian and unitary.
   - Student 2: I disagree. The polarizer operators are not unitary because they do not preserve the norm of the state. It makes sense that they do not preserve the norm because the polarizer absorbs a polarization component of the photon state. However, since we are not interested in the component absorbed, it is OK to consider these polarizer operators in our analysis even though they are not unitary, time-evolution operators.
   - Student 3: We can also check unitarity by $\hat{U}^{\dagger}\hat{U} = \hat{I}$, where $\hat{U}^{\dagger}$ is the hermitian conjugate of the operator $\hat{U}$. We will find that polarizer operators will, in general, not satisfy this relation.
   - Student 4: There is no particular reason for the polarizer operators to be hermitian either because they do not correspond to a physical observable, e.g., position, momentum, energy, etc. If a polarizer operator turns out to be hermitian in a given case, it is just a fluke.

   With whom do you agree? Explain your reasoning.

25. Checkpoint: Matrix representations of basis vectors and operators corresponding to BS1, BS2, mirrors, phase shifter, and polarizers

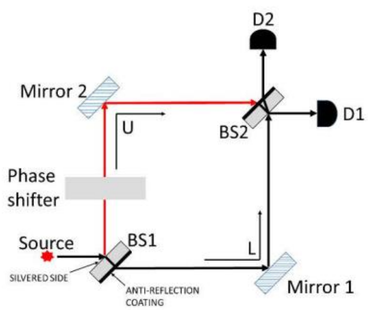
Basis vector	Matrix representation of the basis vector
$\lvert UV\rangle = \lvert U\rangle\lvert V\rangle = \lvert U\rangle\otimes\lvert V\rangle$	$\begin{pmatrix}1\\0\\0\\0\end{pmatrix}$
$\lvert UH\rangle = \lvert U\rangle\lvert H\rangle = \lvert U\rangle\otimes\lvert H\rangle$	$\begin{pmatrix}0\\1\\0\\0\end{pmatrix}$
$\lvert LV\rangle = \lvert L\rangle\lvert V\rangle = \lvert L\rangle\otimes\lvert V\rangle$	$\begin{pmatrix}0\\0\\1\\0\end{pmatrix}$
$\lvert LH\rangle = \lvert L\rangle\lvert H\rangle = \lvert L\rangle\otimes\lvert H\rangle$	$\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$

Operator	Matrix Representation of the operator in the product space including both the path and polarization states
$[BS1]$	$\frac{1}{\sqrt{2}}\begin{bmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$
$[BS2]$	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$
$Mirrors\ [M]$	$\begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$

	Matrix representation of operator involving the upper path	Matrix representation of operator involving the lower path
$[PS]$	$[PS_U] = \begin{bmatrix} e^{i\varphi_{ps}} & 0 & 0 & 0 \\ 0 & e^{i\varphi_{ps}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$	$[PS_L] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{i\varphi_{ps}} & 0 \\ 0 & 0 & 0 & e^{i\varphi_{ps}} \end{bmatrix}$
$[P_V]$	$[P_{UV}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$	$[P_{LV}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$
$[P_H]$	$[P_{UH}] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$	$[P_{LH}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
$[P_{+45°}]$	$[P_{U_{+45°}}] = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$	$[P_{L_{+45°}}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$
$[P_{-45°}]$	$[P_{U_{-45°}}] = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$	$[P_{L_{-45°}}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$

C. **Find the effect of the quantum mechanical operators on an input state of a photon and the probability of a detector D1 or D2 clicking (and registering a photon) when the source emits +45° polarized photons**

i. **Original MZI setup with a phase shifter in the upper path**



- We will now find the action of BS1, mirrors, phase shifter in the upper path, and BS2 on the state of a single 45° polarized photon emitted from the source in the upper path state U, i.e.,

$|U\rangle \otimes |45°\rangle = |U, +45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix}$, as shown in the figure above.

26. Predict the photon state just before the mirrors after it has <u>propagated through BS1</u>, i.e., $[BS1]|U, +45°\rangle$ and select one of the following answers that matches your prediction.

(a) $A\begin{pmatrix}1\\0\\1\\0\end{pmatrix}$, where A is a normalization constant.

(b) $A\begin{pmatrix}-1\\-1\\0\\0\end{pmatrix}$, where A is a normalization constant.

(c) $A\begin{pmatrix}1\\1\\1\\1\end{pmatrix}$, where A is a normalization constant.

(d) $A\begin{pmatrix}-1\\-1\\1\\1\end{pmatrix}$, where A is a normalization constant.

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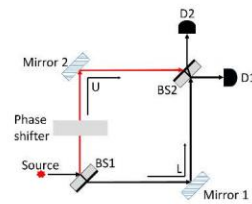
27. Consider the following conversation between two students when the source emits +45° polarized photons:



- Student 1: The photon state <u>after it has propagated through BS1</u> should be a superposition of the upper and lower path states, i.e., $A(-|U,+45°\rangle + |L,+45°\rangle)$, where A is a normalization constant. Since the upper path state is phase shifted by π, it should be multiplied by $e^{i\pi} = -1$. The lower path state is not phase shifted. Also, BS1 does not affect the photon polarization, so the photon remains +45° polarized after passing through BS1.
- Student 2: I disagree. The photon state after it has propagated through BS1 should be $A\begin{pmatrix}-1\\-1\\1\\1\end{pmatrix}$, where A is a normalization constant.
- Student 3: You are both saying the same thing because a +45° polarized photon in the upper path is represented mathematically as $|U,+45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix}$. A +45° polarized photon in the lower path is represented mathematically as $|L,+45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\0\\1\\1\end{pmatrix}$. Thus,

$$A(-|U,+45°\rangle + |L,+45°\rangle) = A\left(-\begin{pmatrix}1\\1\\0\\0\end{pmatrix}+\begin{pmatrix}0\\0\\1\\1\end{pmatrix}\right) = A\begin{pmatrix}-1\\-1\\1\\1\end{pmatrix}, \text{ where } A = \frac{1}{\sqrt{2}}.$$

With whom do you agree?

28. $[BS1]|U,+45°\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}-1 & 0 & 1 & 0\\ 0 & -1 & 0 & 1\\ 1 & 0 & 1 & 0\\ 0 & 1 & 0 & 1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix} = \frac{1}{2}\begin{pmatrix}-1\\-1\\1\\1\end{pmatrix}$. Describe in words what this output represents.

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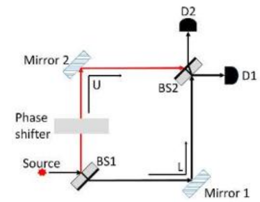
29. Predict the state of the photon just before BS2 after it has propagated through BS1, the mirrors, and the phase shifter in the upper path and select one of the following answers that matches your prediction.



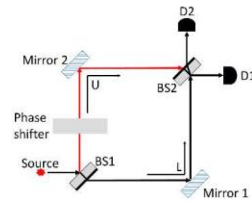
(a) $A\begin{pmatrix} e^{i\varphi_{PS}} \\ e^{i\varphi_{PS}} \\ 1 \\ 1 \end{pmatrix}$, where A is a normalization constant.

(b) $A\begin{pmatrix} -e^{i\varphi_{PS}} \\ -e^{i\varphi_{PS}} \\ 1 \\ 1 \end{pmatrix}$, where A is a normalization constant.

(c) $A\begin{pmatrix} e^{i\varphi_{PS}} \\ e^{i\varphi_{PS}} \\ -1 \\ -1 \end{pmatrix}$, where A is a normalization constant.

(d) $A\begin{pmatrix} 0 \\ -e^{i\varphi_{PS}} \\ 1 \\ 1 \end{pmatrix}$, where A is a normalization constant.

30. The correct answer to the previous question is (c), in which $A = 1/2$. After the photon exits BS2, the final state of the photon is



$$[BS2]\frac{1}{2}\begin{pmatrix} e^{i\varphi_{PS}} \\ e^{i\varphi_{PS}} \\ -1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}\frac{1}{2}\begin{pmatrix} e^{i\varphi_{PS}} \\ e^{i\varphi_{PS}} \\ -1 \\ -1 \end{pmatrix} = \frac{1}{2\sqrt{2}}\begin{pmatrix} e^{i\varphi_{PS}} + 1 \\ e^{i\varphi_{PS}} + 1 \\ e^{i\varphi_{PS}} - 1 \\ e^{i\varphi_{PS}} - 1 \end{pmatrix}$$

$$= \frac{(e^{i\varphi_{PS}} + 1)|U\rangle|V\rangle + (e^{i\varphi_{PS}} + 1)|U\rangle|H\rangle + (e^{i\varphi_{PS}} - 1)|L\rangle|V\rangle + (e^{i\varphi_{PS}} - 1)|L\rangle|H\rangle}{2\sqrt{2}}$$

Consider the following statement about the photon state $\frac{1}{2\sqrt{2}}\begin{pmatrix} e^{i\varphi_{PS}} + 1 \\ e^{i\varphi_{PS}} + 1 \\ e^{i\varphi_{PS}} - 1 \\ e^{i\varphi_{PS}} - 1 \end{pmatrix}$ in the product space of both the path and polarization states.

- Student 1: The photon state $\frac{1}{2\sqrt{2}}\begin{pmatrix} e^{i\varphi_{PS}} + 1 \\ e^{i\varphi_{PS}} + 1 \\ e^{i\varphi_{PS}} - 1 \\ e^{i\varphi_{PS}} - 1 \end{pmatrix}$ is equivalent to $\frac{(e^{i\varphi_{PS}}+1)|U\rangle|V\rangle+(e^{i\varphi_{PS}}+1)|U\rangle|H\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|V\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|H\rangle}{2\sqrt{2}}$ because we have chosen our basis vectors to be $|U\rangle|V\rangle = |UV\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$, $|U\rangle|H\rangle = |UH\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$, $|L\rangle|V\rangle = |LV\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$, and $|L\rangle|H\rangle = |LH\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$.

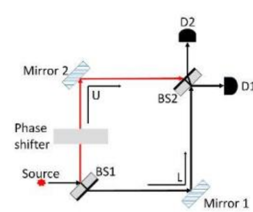
  Therefore,

  $$\frac{1}{2\sqrt{2}}\begin{pmatrix} e^{i\varphi_{PS}} + 1 \\ e^{i\varphi_{PS}} + 1 \\ e^{i\varphi_{PS}} - 1 \\ e^{i\varphi_{PS}} - 1 \end{pmatrix} = \left(\frac{e^{i\varphi_{PS}}+1}{2\sqrt{2}}\right)\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \left(\frac{e^{i\varphi_{PS}}+1}{2\sqrt{2}}\right)\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} + \left(\frac{e^{i\varphi_{PS}}-1}{2\sqrt{2}}\right)\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} + \left(\frac{e^{i\varphi_{PS}}-1}{2\sqrt{2}}\right)\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} =$$

  $$\frac{(e^{i\varphi_{PS}}+1)|U\rangle|V\rangle+(e^{i\varphi_{PS}}+1)|U\rangle|H\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|V\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|H\rangle}{2\sqrt{2}}.$$

Do you agree with student 1?

In the figure to the right, the final state of the photon before it reaches the detectors is



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$|\Psi\rangle = \frac{(e^{i\varphi_{PS}}+1)|U\rangle|V\rangle+(e^{i\varphi_{PS}}+1)|U\rangle|H\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|V\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|H\rangle}{2\sqrt{2}}$.

Detector D1 projects the component of the photon state along the U path. Thus, the total probability of detector D1 registering a photon is

$\left|\frac{(e^{i\varphi_{PS}}+1)}{2\sqrt{2}}\right|^2 + \left|\frac{(e^{i\varphi_{PS}}+1)}{2\sqrt{2}}\right|^2 = \frac{1+\cos\varphi_{PS}}{2}$.

Detector D2 projects the component of the photon state along the L path. Thus, the total probability of detector D2 registering a photon is $\left|\frac{(e^{i\varphi_{PS}}-1)}{2\sqrt{2}}\right|^2 + \left|\frac{(e^{i\varphi_{PS}}-1)}{2\sqrt{2}}\right|^2 = \frac{1-\cos\varphi_{PS}}{2}$.

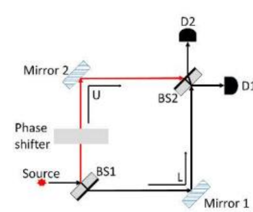
31. Consider the following conversation between two students:
   - Student A: To find the total probability of detector D1 clicking above, we must square the coefficients of the $|U\rangle|V\rangle$ and $|U\rangle|H\rangle$ basis states and add them. We have chosen a basis for the polarization subspace to be $|V\rangle$, $|H\rangle$. The total probability of detector D1 clicking would depend on what polarization basis we choose.
   - Student B: No. The total probability of detector D1 registering a photon does not depend on what polarization basis we choose. Even if you write the state $|\Psi\rangle$ of the photon above in terms of another orthogonal polarization basis, e.g., $|U\rangle|+45°\rangle$ and $|U\rangle|-45°\rangle$, we would obtain the same total probability.

   Predict which student is correct. Write the $|U\rangle|V\rangle$ and $|U\rangle|H\rangle$ states in terms of $|U\rangle|+45°\rangle$ and $|U\rangle|-45°\rangle$ in state $|\Psi\rangle$ in the product space above. Then, square the coefficients and add them to obtain the total probability of detector D1 registering a photon. Is your result consistent with your prediction? If not, reconcile the difference between your prediction and result.

32. Consider the following conversation between two students:
   - Student A: The probability that detector D1 registers a photon is $\frac{1+\cos\varphi_{PS}}{2}$. But what about the polarization state of the photon when it is registered at detector D1? Is the photon detected a horizontally polarized photon, a vertically polarized photon, or neither?
   - Student B: Actually, the polarization of the photon is not well defined, i.e., when detector D1 clicks, the photon is in a superposition of vertical and horizontal polarizations. We have made a partial measurement of path state because detector D1 projects the lower path. But we cannot tell what type of polarization the photon has when it was detected in detector D1. If you also want to measure polarization, you must place a polarizer in front of detector D1.

   Do you agree with Student B's explanation? Explain your reasoning.

33. Consider the following conversation between two students, assuming that Student B was correct in the previous question:



- Student A: Let's cover detector D1 in the upper path with a horizontal polarizer. Now we can measure both the path state and polarization state of the photon. The probability that detector D1 in the lower path registers a horizontally polarized photon is

$$\left|\langle UH|\frac{(e^{i\varphi_{PS}}+1)|U\rangle|V\rangle+(e^{i\varphi_{PS}}+1)|U\rangle|H\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|V\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|H\rangle}{2\sqrt{2}}\right|^2 =$$

$$\left|\frac{(e^{i\varphi_{PS}}+1)}{2\sqrt{2}}\right|^2 = \frac{1+\cos\varphi_{PS}}{4}$$

- Student B: I see. And if we want to determine the probability that detector D1 in the upper path registers a vertically polarized photon, we would place a vertical polarizer in front of detector D1. The probability that detector D1 registers a vertically polarized photon is

$$\left|\langle UV|\frac{(e^{i\varphi_{PS}}-1)|U\rangle|V\rangle+(e^{i\varphi_{PS}}-1)|U\rangle|H\rangle+(e^{i\varphi_{PS}}+1)|L\rangle|V\rangle+(e^{i\varphi_{PS}}+1)|L\rangle|H\rangle}{2\sqrt{2}}\right|^2 =$$

$$\left|\frac{(e^{i\varphi_{PS}}+1)}{2\sqrt{2}}\right|^2 = \frac{1+\cos\varphi_{PS}}{4}$$

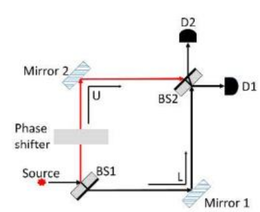
- Student A: And notice that when you add the two probabilities together, you get the total probability of detector D1 registering a photon, $\frac{1+\cos\varphi_{PS}}{2}$. This makes sense because we chose two orthogonal polarization basis states, $|V\rangle$ and $|H\rangle$, in which to make measurements.

Do you agree with the students? Explain your reasoning.

34. Consider the following conversation between two students:
    - Student A: If the total probability of detector D1 registering a photon in the figure shown is $\frac{1+\cos\varphi_{PS}}{2}$, what does this tell us about whether or not we have "which-path" information?
    - Student B: In this case, we don't have "which-path" information since the probability $\frac{1+\cos\varphi_{PS}}{2}$ depends on the phase difference of the photon state from the two paths φ_{PS}. This means that the single photon interferes with itself. BS2 evolves the superposition state of the photon in such a way that the photon state from both U and L paths can be projected by each detector. Thus, when a photon arrives at a detector, the phase difference between the U and L paths in the superposition state at a detector will lead to interference of the photon with itself.

    Do you agree with Student B's explanation? Explain your reasoning.

35. Suppose the phase shifter is removed ($\varphi_{PS}=0$). What is the total probability that detector D1 clicks? Is this probability consistent with what you learned in the earlier part of the Mach Zehnder Interferometer tutorial (Recall that without the phase shifter, detector D1 corresponds to constructive interference in the given setup)?

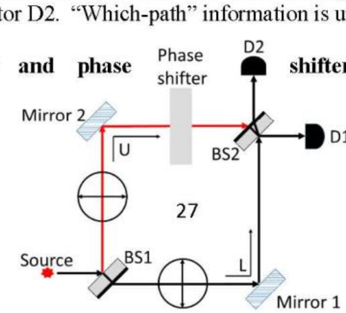


36. Suppose the phase shifter is removed and $\varphi_{PS} = 0$. What is the total probability that detector D2 clicks? Is this probability consistent with what you learned in the earlier part of the Mach Zehnder Interferometer tutorial (Recall that without the phase shifter, detector D2 corresponds to destructive interference in the given setup)?

❖ **Checkpoint**

- In the original MZI setup with a phase shifter in one of the paths and the source emits +45° polarized photons:
  - The probabilities of detector D1 and D2 clicking depend on the phase angle of the phase shifter. "Which-path" information is unknown and interference is displayed.
  - The total probability of detector D1 registering a photon is $\frac{1+\cos\varphi_{PS}}{2}$. If detector D1 is covered by horizontal polarizer, the probability of detector D1 registering a horizontally polarized photon is $\frac{1+\cos\varphi_{PS}}{4}$. If detector D1 is covered by a vertical polarizer, the probability of detector D1 registering a vertically polarized photon is $\frac{1+\cos\varphi_{PS}}{4}$.
  - The total probability of detector D2 registering a photon is $\frac{1-\cos\varphi_{PS}}{2}$. If detector D2 is covered by horizontal polarizer, the probability of detector D2 registering a horizontally polarized photon is $\frac{1-\cos\varphi_{PS}}{4}$. If detector D2 is covered by a vertical polarizer, the probability of detector D1 registering a vertically polarized photon is $\frac{1-\cos\varphi_{PS}}{4}$.
  - If the phase shifter is removed, detector D1 will register a photon emitted from the source with 100% probability. Constructive interference is observed at detector D1. "Which-path" information is unknown and interference is displayed.
  - If the phase shifter is removed, detector D2 will never register a photon. Destructive interference is observed at detector D2. "Which-path" information is unknown and interference is displayed.

ii. Horizontal polarizer and phase shifter in upper path and vertical polarizer in lower path



- We will now find the action of BS1, horizontal polarizer in the upper path, vertical polarizer in the lower path, mirror, phase shifter in the upper path, and BS2 as shown in the figure above on a single 45° polarized photon emitted from the source in the upper path state, i.e., $|U\rangle \otimes |45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix}$.

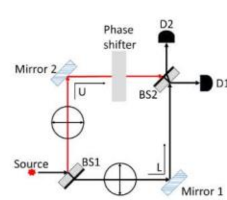
37. Consider the following conversation between two students:
    - Student 1: When we act on the photon state with a vertical polarizer in the lower path and a horizontal polarizer in the upper path as shown above, to find out how the state evolves we can use the matrices corresponding to the polarizer operators we found previously, i.e., $[P_{LV}]$ and $[P_{UH}]$.
    - Student 2: I agree with you. But we can also combine the two matrices $[P_{LV}]$and $[P_{UH}]$ into one matrix by multiplying them, $[P_{LV}] \cdot [P_{UH}]$, since the vertical polarizer operator in the lower path and horizontal polarizer operator in the upper path commute with one another. Then, we can act on the single photon state after the photon passes through BS1 with the combined matrix $[P_{LV}] \cdot [P_{UH}] = [P_{LV}P_{UH}]$, which is equivalent to acting on the photon state with $[P_{LV}]$and $[P_{UH}]$ separately one after another in any order.

    Do you agree with Student 2's explanation? Explain your reasoning.

38. Consider the following conversation between two students:
    - Student 1: In the setup shown above, would varying the thickness of the phase shifter affect how many photons arrive at the detectors?
    - Student 2: No. Since we have "tagged" the photons by placing orthogonal polarizers in the U and L paths, we have "which-path" information about the photon when it is registered at a detector. It is useless to calculate the phase difference between the photon state from the U and L paths for information about interference because we have "which-path" information about each photon that arrives at detectors D1 or D2.
    - Student 3: I agree with you. And the probability for a detector registering a photon will not depend on the phase of the phase shifter. Each detector will register a photon with equal probability.

    Do you agree with Student 2 and Student 3? Explain your reasoning.

39. In the preceding question, Student 2 and Student 3 are correct in their predictions. We will now verify their statements. In the figure shown, predict the state of the photon just



before BS2 after it has propagated through BS1, horizontal polarizer in the upper path and vertical polarizer in the lower path, mirrors, and phase shifter in upper path and select one of the following answers that match your prediction.

(a) $A\begin{pmatrix} 0 \\ -e^{i\varphi_{PS}} \\ 1 \\ 0 \end{pmatrix}$, where A is a normalization constant.

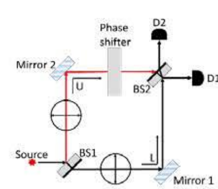
(b) $A\begin{pmatrix} -e^{i\varphi_{PS}} \\ 0 \\ 0 \\ 1 \end{pmatrix}$, where A is a normalization constant.

(c) $A\begin{pmatrix} 0 \\ -e^{i\varphi_{PS}} \\ 1 \\ 0 \end{pmatrix}$, where A is a normalization constant.

(d) $A\begin{pmatrix} 0 \\ e^{i\varphi_{PS}} \\ -1 \\ 0 \end{pmatrix}$, where A is a normalization constant.

40. The correct answer to the previous question is (d), in which $A = 1/2$ which you can find by acting on the initial state with the "time-evolution" operators in this order: $[PS_U][M][P_{LV}P_{UH}][BS1]|U\rangle|45°\rangle$. Describe in words what the mathematical output in the preceding question represents.

41. After the photon exits BS2, the state of the photon is



$|\Psi\rangle = [BS2][PS_U][M][P_{LV}P_{UH}][BS1]|U\rangle|45°\rangle =$

$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0 & -1 & 0\\ 0 & 1 & 0 & -1\\ 1 & 0 & 1 & 0\\ 0 & 1 & 0 & 1\end{bmatrix}\begin{bmatrix}e^{i\varphi_{PS}} & 0 & 0 & 0\\ 0 & e^{i\varphi_{PS}} & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}\begin{bmatrix}-1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\end{bmatrix}\begin{bmatrix}0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}-1 & 0 & 1 & 0\\ 0 & -1 & 0 & 1\\ 1 & 0 & 1 & 0\\ 0 & 1 & 0 & 1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix} =$$

$$|\Psi\rangle = \frac{1}{2\sqrt{2}}\begin{pmatrix}1\\ e^{i\varphi_{PS}}\\ -1\\ e^{i\varphi_{PS}}\end{pmatrix}.$$

(a) Which one of the following correctly describes the photon state $\frac{1}{2\sqrt{2}}\begin{pmatrix}1\\ e^{i\varphi_{PS}}\\ -1\\ e^{i\varphi_{PS}}\end{pmatrix}$ as given above?

i. $\frac{1}{2\sqrt{2}}\begin{pmatrix}1\\ e^{i\varphi_{PS}}\\ -1\\ e^{i\varphi_{PS}}\end{pmatrix} = \frac{|U\rangle|V\rangle - e^{i\varphi_{PS}}|U\rangle|H\rangle + |L\rangle|V\rangle + e^{i\varphi_{PS}}|L\rangle|H\rangle}{2\sqrt{2}}$

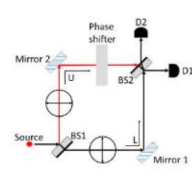
ii. $\frac{1}{2\sqrt{2}}\begin{pmatrix}1\\ e^{i\varphi_{PS}}\\ -1\\ e^{i\varphi_{PS}}\end{pmatrix} = \frac{-|U\rangle|V\rangle + e^{i\varphi_{PS}}|U\rangle|H\rangle + |L\rangle|H\rangle + e^{i\varphi_{PS}}|L\rangle|V\rangle}{2\sqrt{2}}$

iii. $\frac{1}{2\sqrt{2}}\begin{pmatrix}1\\ e^{i\varphi_{PS}}\\ -1\\ e^{i\varphi_{PS}}\end{pmatrix} = \frac{-|L\rangle|V\rangle + e^{i\varphi_{PS}}|L\rangle|H\rangle + |U\rangle|V\rangle + e^{i\varphi_{PS}}|U\rangle|H\rangle}{2\sqrt{2}}$

iv. $\frac{1}{2\sqrt{2}}\begin{pmatrix}1\\ e^{i\varphi_{PS}}\\ -1\\ e^{i\varphi_{PS}}\end{pmatrix} = \frac{|U\rangle|V\rangle + e^{i\varphi_{PS}}|U\rangle|H\rangle - |L\rangle|V\rangle + e^{i\varphi_{PS}}|L\rangle|H\rangle}{2\sqrt{2}}$

(b) Based upon your answer to the previous part, what is the total probability of detector D1 clicking and registering a photon (if it is not covered by a polarizer)? Does the probability depend on the phase shifter?

(c) If detector D1 in the upper path is covered by a vertical polarizer, what is the probability that detector D1 clicks and registers a vertically polarized photon? If detector D1 is covered by a horizontal polarizer, what is the probability that detector D1 clicks and registers a horizontally polarized photon?



(d) What is the total probability that detector D2 clicks (if it is not covered by a polarizer)? Does the probability depend on the phase shift of the phase shifter?

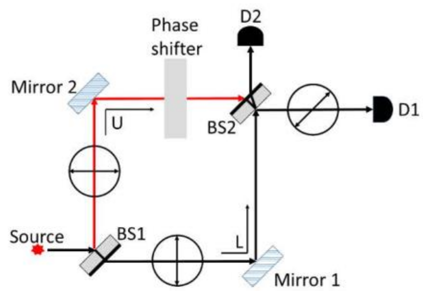
(e) If detector D2 in the lower path is covered by a vertical polarizer, what is the probability that detector D2 clicks and registers a vertically polarized photon? If detector D2 is covered by a horizontal polarizer, what is the probability that detector D2 clicks and registers a horizontally polarized photon?

(f) Suppose the phase shifter is removed ($\varphi_{PS} = 0$). What is the final state of the photon right before the detectors? What is the total probability that detector D1 clicks? What is the total probability that detector D2 clicks? Are these probabilities consistent with what you learned in the earlier part of the Mach Zehnder Interferometer tutorial. (Recall that when there are two orthogonal polarizers in the U and L paths, we have "which-path" information about all photons.)

- **Checkpoint**
  - If a horizontal polarizer and phase shifter are placed in upper path and vertical polarizer is placed in lower path of the MZI and the source emits +45° polarized photons:
    - The probabilities of detector D1 and D2 clicking do not depend on the phase angle of the phase shifter. "Which-path" information is known and interference is not displayed.
    - The total probability of detector D1 registering a photon emitted from the source is 25%.
    - The total probability of detector D2 registering a photon emitted from the source is 25%.

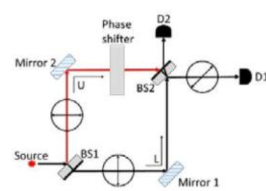
- If the phase shifter is removed, the total probability of detector D1 registering a photon emitted from the source is 25%. The total probability of detector D2 registering a photon emitted from the source is 25%.

iii. **QUANTUM ERASER with a horizontal polarizer in the upper path, vertical polarizer in the lower path, phase shifter in the upper path, and +45° polarizer placed in the lower path between BS2 and detector D1**



- We will now find the action of BS1, horizontal polarizer in the upper path, vertical polarizer in the lower path, mirror, phase shifter in the upper path, BS2, and a 45° polarizer in the lower path (between BS2 and detector D1) on a single 45° polarized photon emitted from the source in the upper path state shown above, i.e., when $|U\rangle \otimes |45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix}$ is the initial state of the photon emitted from the source.
- The MZI setup shown above is a <u>quantum eraser</u> because the +45° polarizer before detector D1 erases "which-path" information about the photon arriving at detector D1. In the following questions, you will check this erasure of "which-path" information due to the 45° polarizer mathematically.

42. Predict the state of the photon just before BS2 after it has <u>propagated through BS1, the polarizers, mirrors, and the phase shifter in the upper path</u> and select one of the following answers that match your prediction.



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(a) $A\begin{pmatrix} 0 \\ e^{i\varphi_{PS}} \\ 1 \\ 0 \end{pmatrix}$, where A is a normalization constant.

(b) $A\begin{pmatrix} 0 \\ -e^{i\varphi_{PS}} \\ 1 \\ 0 \end{pmatrix}$, where A is a normalization constant.

(c) $A\begin{pmatrix} 0 \\ e^{i\varphi_{PS}} \\ -1 \\ 0 \end{pmatrix}$, where A is a normalization constant.

(d) $A\begin{pmatrix} 0 \\ -e^{i\varphi_{PS}} \\ -1 \\ 0 \end{pmatrix}$, where A is a normalization constant.

43. The state of the photon after it has <u>propagated through BS1, the polarizers, mirrors, and the phase shifter in the upper path</u> is $\frac{1}{2}\begin{pmatrix} 0 \\ e^{i\varphi_{PS}} \\ -1 \\ 0 \end{pmatrix}$. In terms of the product space of path states and polarization states, what is $\frac{1}{2}\begin{pmatrix} 0 \\ e^{i\varphi_{PS}} \\ -1 \\ 0 \end{pmatrix}$, where basis vectors are chosen in the order $|UV\rangle$, $|UH\rangle$, $|LV\rangle$, and $|LH\rangle$?

(a) $\frac{e^{i\varphi_{PS}}|U\rangle|V\rangle - |L\rangle|V\rangle}{2}$

(b) $\frac{e^{i\varphi_{PS}}|U\rangle|H\rangle - |L\rangle|H\rangle}{2}$

(c) $\frac{e^{i\varphi_{PS}}|U\rangle|H\rangle - |U\rangle|V\rangle}{2}$

(d) $\frac{e^{i\varphi_{PS}}|U\rangle|H\rangle - |L\rangle|V\rangle}{2}$

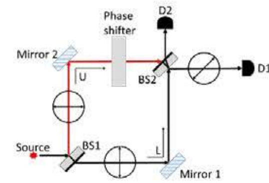
44. The correct answer to the preceding question is (d). For the setup shown above, the final state of the photon is

$$|\Psi\rangle = [P_{U_{+45^\circ}}][BS2][PS_U][M][P_{LV}P_{UH}][BS1]|U\rangle|45^\circ\rangle =$$

$$\frac{1}{2\sqrt{2}}\begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}\begin{bmatrix} e^{i\varphi_{PS}} & 0 & 0 & 0 \\ 0 & e^{i\varphi_{PS}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}\begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$= \frac{1}{2\sqrt{2}}\begin{pmatrix} (\frac{1}{2} + \frac{1}{2}e^{i\varphi_{PS}}) \\ (\frac{1}{2} + \frac{1}{2}e^{i\varphi_{PS}}) \\ -1 \\ e^{i\varphi_{PS}} \end{pmatrix} = \frac{\left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)|U\rangle|V\rangle + \left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)|U\rangle|H\rangle - |L\rangle|V\rangle + e^{i\varphi_{PS}}|L\rangle|H\rangle}{2\sqrt{2}}.$$

(a) Consider the following conversation between two students about the output shown above:



- Student 1: The total probability of detector D1 registering a photon is $\left|\frac{\left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)}{2\sqrt{2}}\right|^2 + \left|\frac{\left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)}{2\sqrt{2}}\right|^2 = \frac{1+\cos\varphi_{PS}}{8}$ since detector D1 projects the component of the photon state along the U path.
- Student 2: I agree. If detector D1 in the lower path is covered by a vertical polarizer, the probability of detector D1 registering a vertically polarized photon is $|\langle UV|\Psi\rangle|^2$, in which $|\Psi\rangle$ is the final state of the photon given above. Thus,

$$\left|\langle UV|\left(\frac{\left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)|U\rangle|V\rangle+\left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)|U\rangle|H\rangle-|L\rangle|V\rangle+e^{i\varphi_{PS}}|L\rangle|H\rangle}{2\sqrt{2}}\right)\right|^2 = \left|\frac{\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}}{2\sqrt{2}}\right|^2 = \frac{1+\cos\varphi_{PS}}{16}.$$

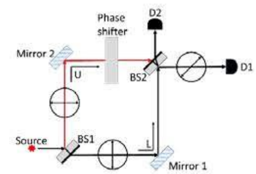
And if detector D1 is covered by a horizontal polarizer, the probability of detector D1 registering a horizontally polarized photon is $|\langle UH|\Psi\rangle|^2$, where $|\Psi\rangle$ is the final state of the photon shown above. Thus,

$$\left|\langle UH|\left(\frac{\left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)|U\rangle|V\rangle+\left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)|U\rangle|H\rangle-|L\rangle|V\rangle+e^{i\varphi_{PS}}|L\rangle|H\rangle}{2\sqrt{2}}\right)\right|^2 = \left|\frac{\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}}{2\sqrt{2}}\right|^2 = \frac{1+\cos\varphi_{PS}}{16}.$$

Do you agree with Student 1 and Student 2? Explain your reasoning.

(b) Does the <u>total probability</u> that detector D1 "clicks" (and registers a photon) in the preceding question depend on the phase shift of the phase shifter, e.g., changing the thickness of the piece of glass? In particular, as we gradually change the thickness of the glass piece, will we observe the probability of registering a photon at detector D1 change? Explain your reasoning.

(c) Is "which-path" information known about the photon when detector D1 "clicks" in the preceding question? Explain your reasoning.



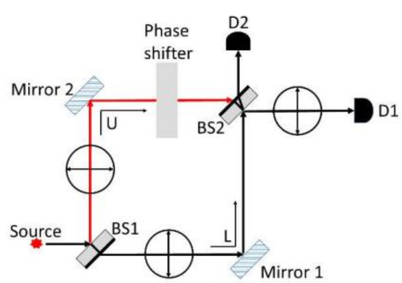
(d) What is the total probability that detector D2 registers a photon if detector D2 is not covered by a polarizer in the preceding question?

(e) In the figure shown to the right, does the probability that detector D2 "clicks" (and registers a photon) depend on the phase shift of the phase shifter, e.g., changing the thickness of the piece of glass? Explain your reasoning.

(f) Is "which-path" information known about the photon when detector D2 "clicks"? Explain your reasoning.

(g) In the figure shown above, suppose the phase shifter is removed ($\varphi_{PS} = 0$). What is the final state of the photon right before detector D1 and D2? What is the total probability that detector D1 clicks (and registers a photon) if detector D1 is not covered a polarizer? What is the total probability that detector D2 clicks (and registers a photon) if detector D2 is not covered by a polarizer? Is this probability consistent with what you learned in the earlier part of the Mach Zehnder Interferometer tutorial?

- ❖ **Checkpoint**
  - **In the quantum eraser setup in which the source emits +45° polarized photons:**
    - The total probability of detector D1 registering a photon emitted from the source depends on the phase angle of the phase shifter. "Which-path" information is unknown and interference is displayed at detector D1.
    - The total probability of detector D1 registering a photon is $\frac{1+\cos\varphi_{PS}}{8}$. If detector D1 is covered by a horizontal polarizer, the probability of detector D1 registering a horizontally polarized photon is $\frac{1+\cos\varphi_{PS}}{16}$. If detector D1 is covered by a vertical polarizer, the probability of detector D1 registering a vertically polarized photon is $\frac{1+\cos\varphi_{PS}}{16}$.
    - The total probability of detector D2 registering a photon emitted from the source is 25% and does NOT depend on the phase angle of the phase shifter. "Which-path" information is known and interference is not displayed.



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45. Consider the following conversation about the MZI setup shown above.

- Student 1: Is the setup above still a quantum eraser setup?
- Student 2: No. If we change the polarization of the 45° polarizer to 90°, the final state of the photon is $[P_{UV}][BS2][PS_U][M][P_{LV}P_{UH}][BS1]|U\rangle|45°\rangle = \frac{|U\rangle|V\rangle - |L\rangle|V\rangle + e^{i\varphi_{PS}}|L\rangle|H\rangle}{2\sqrt{2}}$. Only the vertical component of the photon state from the lower path can be projected in detector D1. So that setup is not a quantum eraser.
- Student 3: However, if the polarization axis of the 45° polarizer was changed to 30°, it would absorb some photons but allow some photons to pass through (fewer than if the polarization axis was at 45°). Thus, we can project the photon components from the U and L path states into detector D1 and we do not have "which-path" information for the photon. Thus, this setup would be a quantum eraser. Interference will be observed at detector D1.

Do you agree with Student 2 and student 3's explanations? Explain your reasoning.

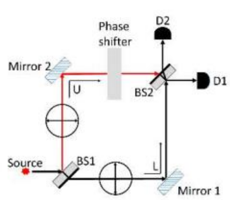


Figure 1

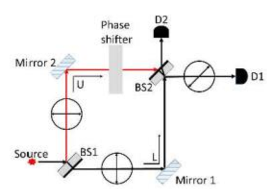


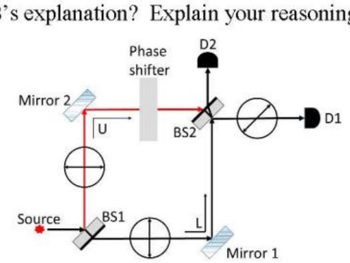
Figure 2

46. Consider the following conversation between two students about the MZI setups shown above.

- Student A: The final state of the photon in figure 1 is $\frac{|U\rangle|V\rangle + e^{i\varphi_{PS}}|U\rangle|H\rangle - |L\rangle|V\rangle + e^{i\varphi_{PS}}|L\rangle|H\rangle}{2\sqrt{2}}$ and the final state of the photon in figure 2 is $\frac{\left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)|U\rangle|V\rangle + \left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)|U\rangle|H\rangle - |L\rangle|V\rangle + e^{i\varphi_{PS}}|L\rangle|H\rangle}{2\sqrt{2}}$. How can we tell that figure 1 is not a quantum eraser setup and figure 2 is a quantum eraser by looking at the final state of the photon?

- Student B: In figure 1, the probabilities of a photon arriving at detectors D1 and D2 do not depend on the phase shift of the phase shifter. So of all of the photons that pass through the polarizers, half of them arrive at each detector D1 and D2. In figure 1, since there is no +45° polarizer between BS2 and detector D2, we have "which-path" information for a photon that arrives at detector D2 and we would not observe interference at detector D2. From the expression given above for figure 1, the total probability of the photon arriving at detector D2 is $\left|\frac{1}{2\sqrt{2}}\right|^2 + \left|\frac{e^{i\varphi_{PS}}}{2\sqrt{2}}\right|^2 = \frac{1}{4}$ and does not depend on the phase shift of the phase shifter. On the other hand, in figure 2, the total probability of the photon arriving at detector D1 depends on the phase shift of the phase shifter. So we could observe constructive interference, destructive interference, or intermediate interference at detector D1 depending on the phase shift of the phase shifter.
- Student A: But when the phase shifter is removed ($\varphi_{PS} = 0$), the final states of the photon in each of the figures are the same, $\frac{|U\rangle|V\rangle+|U\rangle|H\rangle-|L\rangle|V\rangle+|L\rangle|H\rangle}{2\sqrt{2}}$. So how can we tell that figure 2 is a quantum eraser case?
- Student B: For the special case $\varphi_{PS} = 0$ when the phase shifter is removed, the states in both figures 1 and 2 look the same and we cannot tell that figure 2 is a quantum eraser if the source is emitting a highly collimated stream of single photons. If the source emits a highly collimated stream of a large number (N) of single photons, then the probability that detector D1 clicks is $\left|\frac{1}{2\sqrt{2}}\right|^2 + \left|\frac{1}{2\sqrt{2}}\right|^2 = \frac{1}{4}$ for both situations (figure 1 and figure 2) for $\varphi_{PS} = 0$. We cannot tell if the 45° polarizer is erasing quantum information just by considering one special case because we cannot tell if there is interference unless we change the phase difference between the two paths and observe that it makes a difference. However, if the source emits a large number (N) of single photons with <u>a transverse Gaussian width</u> and we replace detector D1 with a planar detector (screen) we would be able to tell that figure 2 is a quantum eraser setup. We would see an interference pattern emerge on the planar screen due to the path length differences of the photon with a transverse Gaussian width, as in the computer simulation.

Do you agree with Student B's explanation? Explain your reasoning.



47. In the figure above, suppose the source emits -45° polarized photons, $|U\rangle|-45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\\0\\0\end{pmatrix}$. The final state of the photon is

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$$[P_{U_{+45^\circ}}][BS2][PS_U][M][P_{LV}P_{UH}][BS1]|U\rangle|-45^\circ\rangle$$

$$= \frac{1}{2\sqrt{2}}\begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}\begin{bmatrix} e^{i\varphi_{PS}} & 0 & 0 & 0 \\ 0 & e^{i\varphi_{PS}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}\begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}$$

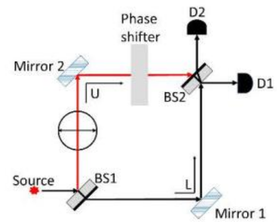
$$= \frac{1}{2\sqrt{2}}\begin{pmatrix} -1 \\ -e^{i\varphi_{PS}} \\ \frac{1}{2} - \frac{1}{2}e^{i\varphi_{PS}} \\ \frac{1}{2} - \frac{1}{2}e^{i\varphi_{PS}} \end{pmatrix} = \frac{\left(\frac{1}{2}-\frac{1}{2}e^{i\varphi_{PS}}\right)|U\rangle|V\rangle + \left(\frac{1}{2}-\frac{1}{2}e^{i\varphi_{PS}}\right)|U\rangle|H\rangle - |L\rangle|V\rangle - e^{i\varphi_{PS}}|L\rangle|H\rangle}{2\sqrt{2}}.$$

(a) What is the total probability that detector D1 registers a photon (assume detector D1 is not covered by a polarizer) in the figure above.

(b) Unpolarized light can be thought of as an equal mixture of 45° polarized photons and -45°polarized photons. To find the total probability of unpolarized photons arriving at detector D1, we can average the total probabilities of detector D1 registering a photon for the two cases in which the source emits +45° single photons and -45° single photons (questions 44 and 47 (a)). Does the probability of unpolarized photons arriving at detector D1 depend on the phase shift of the phase shifter? Does the quantum eraser setup make a distinction between polarized and unpolarized photons (will the quantum eraser work with unpolarized photons)?

- Checkpoint
  - The total probability of unpolarized photons arriving at detector D1 can be determined by averaging the total probabilities of detector D1 registering a photon for the two cases in which the source emits +45° single photons and -45° single photons. The total probability of detector D1 registering a photon when the source emits +45° single photons is $\frac{1+\cos\varphi_{PS}}{8}$ and the total probability of detector D1 registering a photon when the source emits -45° single photons is $\frac{1-\cos\varphi_{PS}}{8}$. The average of these probabilities is $\frac{1}{8}$. Thus, the total probability of unpolarized photons arriving at detector D1 is $\frac{1}{8}$ and does not depend on the phase angle of the phase shifter. "Which-path" information is known and interference is displayed.

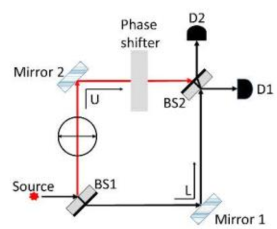
iii. Horizontal polarizer and phase shifter in upper path



- In the figure above, we will now find the action of BS1, horizontal polarizer in the upper path, mirror, phase shifter in upper path, and BS2 on a single 45° polarized photon emitted from the source in the upper path state U, i.e., when $|U\rangle|45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix}$ is the initial state of the photon emitted from the source.

48. For the figure above, predict the output of the photon state just before the phase shifter after the photon has propagated through BS1, the horizontal polarizer in the upper path, and reflected off the mirrors, i.e., what is $[M][P_{UH}][BS1]|U\rangle|45°\rangle$?

49. For the figure shown above, the photon state after the photon propagates through BS1, the horizontal polarizer in the upper path, and the mirrors is $[M][P_{UH}][BS1]|U\rangle|45°\rangle =$
$\begin{bmatrix}-1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix}\begin{bmatrix}0&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}-1&0&1&0\\0&-1&0&1\\1&0&1&0\\0&1&0&1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix} =$
$\frac{1}{2}\begin{pmatrix}0\\1\\-1\\-1\end{pmatrix}$. Describe in words what this output represents.



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50. After the photon propagates through BS1, the horizontal polarizer in the upper path, mirrors, phase shifter in the upper path, and BS2, the photon state in the figure to the right is

$[BS2][PS_U][M][P_{UH}][BS1]|U\rangle|45°\rangle =$

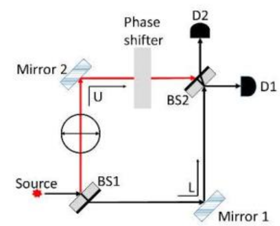
$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0 & -1 & 0\\ 0 & 1 & 0 & -1\\ 1 & 0 & 1 & 0\\ 0 & 1 & 0 & 1\end{bmatrix}\begin{bmatrix}e^{i\varphi_{PS}} & 0 & 0 & 0\\ 0 & e^{i\varphi_{PS}} & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}\begin{bmatrix}-1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\end{bmatrix}\begin{bmatrix}0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}-1 & 0 & 1 & 0\\ 0 & -1 & 0 & 1\\ 1 & 0 & 1 & 0\\ 0 & 1 & 0 & 1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\\ 0\\ 0\end{pmatrix} =$$

$$\frac{1}{2\sqrt{2}}\begin{pmatrix}1\\ e^{i\varphi_{PS}}+1\\ -1\\ e^{i\varphi_{PS}}-1\end{pmatrix} = \frac{|U\rangle|V\rangle+(e^{i\varphi_{PS}}+1)|U\rangle|H\rangle-|L\rangle|V\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|H\rangle}{2\sqrt{2}}.$$

(a) What is the <u>total probability</u> that detector D1 clicks (if not covered by a polarizer)? If detector D1 is covered by a vertical polarizer, what is the probability that detector D1 registers a vertically polarized photon? If detector D1 is covered by a horizontal polarizer, what is the probability that detector D1 registers a horizontally polarized photon?

(b) What is the <u>total probability</u> that detector D2 clicks (if not covered by a polarizer) in the figure shown? If detector D2 is covered by a vertical polarizer, what is the probability that detector D2 registers a vertically polarized photon? If detector D2 is covered by a horizontal polarizer, what is the probability that detector D2 registers a horizontally polarized photon?

(d) For photons with which polarization type do you have "which-path" information? Based on the output $[BS2][PS_U][M][P_{UH}][BS1]|U\rangle|45°\rangle = \frac{|U\rangle|V\rangle+(e^{i\varphi_{PS}}+1)|U\rangle|H\rangle-|L\rangle|V\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|H\rangle}{2\sqrt{2}}$, do these photons have equal probability of arriving at each detector D1 and D2? Explain.

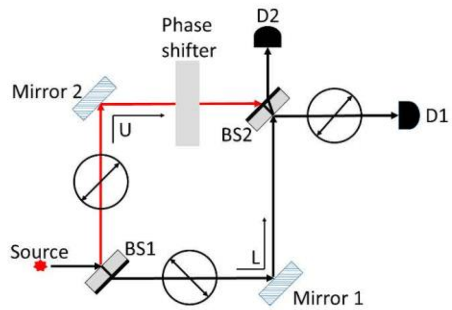


(e) For photons with which polarization type do you NOT have "which-path" information? Based on the output $[BS2][PS_U][M][P_{HU}][BS1]|U\rangle|45°\rangle = \frac{|U\rangle|V\rangle+(e^{i\varphi_{PS}}+1)|U\rangle|H\rangle-|L\rangle|V\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|H\rangle}{2\sqrt{2}}$, do these photons display interference at detectors D1 and D2? Explain.

(f) In the figure shown above, suppose the phase shifter is removed ($\varphi_{PS} = 0$). What is the final state of the photon right before detector D1 and D2? What is the total probability that detector D1 clicks (and registers a photon) if detector D1 is not covered a polarizer? What is the total probability that detector D2 clicks (and registers a photon) if detector D2 is not covered by a polarizer? Is this probability consistent with what you learned in the earlier part of the Mach Zehnder Interferometer tutorial?

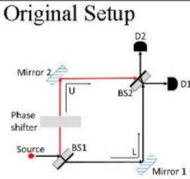
- **Checkpoint**
  - If a Horizontal polarizer and phase shifter are placed in the upper path of the MZI:
    - The total probabilities of detector D1 and D2 registering a photon depend on the phase angle of the phase shifter. "Which-path" information is unknown for horizontally polarized photons and these photons display interference at the detectors. "Which-path" information is known for vertically polarized photons and these photons do not display interference at the detectors.
    - The total probability of detector D1 registering a photon emitted from the source is $\frac{1}{8}+\frac{1+\cos\phi}{4}$.
    - The total probability of detector D2 registering a photon emitted from the source is $\frac{1}{8}+\frac{1-\cos\phi}{4}$.
    - If the phase shifter is removed, the total probability of detector D1 registering a photon emitted from the source is $\frac{5}{8}$ (probability of $1/8$ for registering vertically polarized photons which do not display interference and probability of ½ for registering horizontally polarized photons which

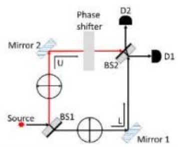
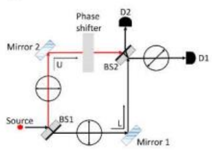
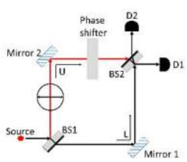
display interference) and the total probability of detector D2 registering a photon emitted from the source is $\frac{1}{8}$ (probability of $1/8$ for registering vertically polarized photons which do not display interference).



51. Bonus question: In the setup shown above, if the source emits 45° polarized single photons, the final state of the photon is
$[P_{U_{+45°}}][BS2][PS_U][M][P_{U_{+45°}}][P_{L_{-45°}}][BS1]|U\rangle|45°\rangle = \frac{e^{i\varphi_{PS}}|U\rangle|V\rangle+e^{i\varphi_{PS}}|U\rangle|H\rangle+e^{i\varphi_{PS}}|L\rangle|V\rangle+e^{i\varphi_{PS}}|L\rangle|H\rangle}{2\sqrt{2}}$.
With what total probabilities do the detectors D1 and D2 register a photon (if they are not covered by polarizers)? Do you have "which-path" information about any photons emitted from the source that arrive at detectors D1 and D2?

Summary

MZI Setup	**Final State of the Photon**	**What is the probability of:** **a) D1 registering a photon?** **b) D2 registering a photon?** **d) Do you have "which-path" information about any of the photons arriving at the detectors?**
Original Setup 	$\frac{(e^{i\varphi_{PS}}+1)|U\rangle|V\rangle+(e^{i\varphi_{PS}}+1)|U\rangle|H\rangle}{2\sqrt{2}}+\frac{(e^{i\varphi_{PS}}-1)|L\rangle|V\rangle+(e^{i\varphi_{PS}}-1)|L\rangle|H\rangle}{2\sqrt{2}}$	a) $\frac{1+\cos\phi}{2}$ b) $\frac{1-\cos\phi}{2}$ c) No "which-path" information. All photons display interference.

Two Orthogonal Polarizers 	$\frac{\lvert U\rangle\lvert V\rangle + e^{i\varphi_{PS}}\lvert U\rangle\lvert H\rangle}{2\sqrt{2}} + \frac{-\lvert L\rangle\lvert V\rangle + e^{i\varphi_{PS}}\lvert L\rangle\lvert H\rangle}{2\sqrt{2}}$	a) $\frac{1}{4}$ b) $\frac{1}{4}$ c) "Which-path" information is known about all photons arriving at the detectors. No photons display interference.
Quantum Eraser 	$\frac{\left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)\lvert U\rangle\lvert V\rangle + \left(\frac{1}{2}+\frac{1}{2}e^{i\varphi_{PS}}\right)\lvert U\rangle\lvert H\rangle}{2\sqrt{2}} + \frac{-\lvert L\rangle\lvert V\rangle + e^{i\varphi_{PS}}\lvert L\rangle\lvert H\rangle}{2\sqrt{2}}$	a) $\frac{1+\cos\phi}{8}$ b) $\frac{1}{4}$ c) "Which-path" information is unknown about all photons arriving at D1. Photons arriving at D1 display interference. "Which-path" information is known about all photons arriving at detector D2. Photons arriving at D2 do not display interference.
Polarizer with horizontal polarization axis in one path of the MZI 	$\frac{\lvert U\rangle\lvert V\rangle + \left(e^{i\varphi_{PS}}+1\right)\lvert U\rangle\lvert H\rangle}{2\sqrt{2}} + \frac{-\lvert L\rangle\lvert V\rangle + (e^{i\varphi_{PS}}-1)\lvert L\rangle\lvert H\rangle}{2\sqrt{2}}$	a) $\frac{1}{8}+\frac{1+\cos\phi}{4}$ b) $\frac{1}{8}+\frac{1-\cos\phi}{4}$ c) "Which-path" information is known about $\frac{1}{8}$ of the photons arriving at detector D1 and they do not display interference. "Which-path" information is unknown about $\frac{1+\cos\phi}{4}$ of the photons arriving at detector D1 and they display interference. "Which-path" information is known about $\frac{1}{8}$ of the photons arriving at detector D2 and they do not display interference. "Which-path" information is unknown about $\frac{1-\cos\phi}{4}$ of the photons arriving at detector D2 and they display interference.

APPENDIX B: ADDITIONAL CLICKER QUESTION SEQUENCES

B.1 IDENTICAL PARTICLES: WAVEFUNCTION SYMMETRY

Identical Particles

Choose all of the following that are true about the Hamiltonian and basis vectors for a system of two non-interacting particles given that the single-particle Hamiltonian is H_i (where i=1,2) and the single-particle wavefunction is $\psi_i(x_i)$:

(1) The total Hamiltonian can be written as the sum of the individual Hamiltonians for each particle, $H_{TOT} = \sum_i H_i$.

(2) For the system of two-particles, $\psi_1(x_1) + \psi_2(x_2)$ or $\psi_1(x_1)\psi_2(x_2)$ are both examples of suitable basis vectors.

(3) The Hamiltonian operator for one of the particles $\widehat{H}_2$ acting on the state $\psi_1(x_1)\psi_2(x_2)$ will return the energy eigenvalue for its respective particle, $\widehat{H}_2\psi_1(x_1)\psi_2(x_2) = E_2\psi_1(x_1)\psi_2(x_2)$.

A. 2 only B. 3 only C. 1 and 2 only D. 1 and 3 only
E. None of the above

Identical Particles

There are three identical spinless fermions in a one dimensional infinite square well. The single particle stationary states are ψ_n (n=1, 2, 3, …where n=1 is the ground state). Choose all of the following statements that are correct for the three particle system.

(1) The ground state of the three particle system is $\psi_1(x_1)\psi_2(x_2)\,\psi_3(x_3)$.

(2) $\psi_1(x_1)\psi_2(x_2)\,\psi_4(x_3)$ is one of the first excited state wavefunctions of the three particle system.

(3) There are 6 distinct wavefunctions of the first excited state with the same energy.

A. 1 only B. 2 only C. 3 only D. 2 and 3 only
E. None of the above.

Identical Particles

There are three identical spinless bosons in a one dimensional infinite square well. The single particle stationary states are ψ_n (n=1, 2, 3, …). Choose all of the following statements that are correct for the three particle system. (**Note: different subscripts in answers choices**)

(1) The ground state of the three particle system is $\psi_1(x_1)\psi_1(x_2)\,\psi_1(x_3)$.

(2) The ground state of the three particle system is $\psi_1(x)\psi_1(x)\,\psi_1(x)$.

(3) $\psi_1(x_1)\psi_1(x_2)\,\psi_2(x_3)$ is one of the first excited state wavefunctions of the three particle system.

A. 1 only B. 2 only C. 3 only D. 2 and 3 only
E. None of the above

Identical Particles

There are three distinguishable particles with the same mass in a one dimensional infinite square well. The single particle stationary states are ψ_n (n=1, 2, 3, …) where n=1 is the lowest energy state. Choose all of the following statements that are correct for the three particle system.

(1) The ground state of the three particle system is $\psi_1(x_1)\psi_1(x_2)\,\psi_1(x_3)$.

(2) $\psi_1(x_1)\psi_1(x_2)\,\psi_2(x_3)$ is one of the first excited state wavefunctions of the three particle system.

(3) There are 6 distinct wavefunctions of the first excited state with the same energy.

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only
E. all of the above

Class Discussion

What are the differences in wavefunctions for fermions, bosons, and the contrasting case of distinguishable particles?

Identical Particles

Choose all of the following wavefunctions that are possible for <u>two "spinless" fermions</u> in a one-dimensional infinite square well with width a. The wavefunction for a single particle in a one-dimensional infinite square well is $\psi_n \sim \sin\left(\frac{n\pi x}{a}\right)$ and "A" is a suitable normalization constant.

(1) $A \sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{a}\right)$
(2) $A \sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{3\pi x_2}{a}\right)$
(3) $A \left[\sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{3\pi x_2}{a}\right) - \sin\left(\frac{3\pi x_1}{a}\right) \sin\left(\frac{2\pi x_2}{a}\right)\right]$

A. 1 only B. 2 only C. 3 only D. 2 and 3 only E. None of the above

Identical Particles

Choose all of the following wavefunctions that are possible for <u>two "spinless" bosons</u> in a one-dimensional infinite square well with width a. Ignore spin. The wavefunction for a single particle in a one-dimensional infinite square well is $\psi_n \sim \sin\left(\frac{n\pi x}{a}\right)$ and "A" is a suitable normalization constant. **(Note sign change in (3))**

(1) $A \sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{a}\right)$
(2) $A \sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{3\pi x_2}{a}\right)$
(3) $A \left[\sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{3\pi x_2}{a}\right) + \sin\left(\frac{3\pi x_1}{a}\right) \sin\left(\frac{2\pi x_2}{a}\right)\right]$

A. 3 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only E. All of the above

Identical Particles

Choose all of the following wavefunctions that are possible for two distinguishable particles in a one-dimensional infinite square well with width a. Ignore spin. The wavefunction for a single particle in a one-dimensional infinite square well is $\psi_n \sim \sin\left(\frac{n\pi x}{a}\right)$ and "A" is a suitable normalization constant.

(1) $A \sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{a}\right)$

(2) $A \sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{3\pi x_2}{a}\right)$

(3) $A \left[\sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{3\pi x_2}{a}\right) + \sin\left(\frac{3\pi x_1}{a}\right) \sin\left(\frac{2\pi x_2}{a}\right)\right]$

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only E. All of the above

Notes on Spin Notations:

- For a pair of spin-1/2 fermions, the uncoupled spin notation will be used as follows:

  $|s_1, m_{s1}\rangle \otimes |s_2, m_{s2}\rangle = \left|\frac{1}{2}, \frac{1}{2}\right\rangle \otimes \left|\frac{1}{2}, \frac{-1}{2}\right\rangle = |\uparrow\downarrow\rangle$
- For a pair of spin-1 bosons, the uncoupled spin notation will be used as follows:

  $|s_1, m_{s1}\rangle \otimes |s_2, m_{s2}\rangle = |1,1\rangle \otimes |1,0\rangle$

Identical Particles

There are two identical **spin-$\frac{1}{2}$ particles** in a one dimensional infinite square well. The single particle stationary states are ψ_n (n=1, 2, 3, …). Choose all of the following statements that are correct for the two particle system.

(1) A ground state of the two particle system is $\psi_1(x_1)\psi_1(x_2)|\uparrow\downarrow\rangle$.

(2) $\psi_1(x_1)\psi_2(x_2)|\uparrow\uparrow\rangle$ is one of the first excited state wavefunctions of the two particle system.

(3) A ground state of the two particle system is $\psi_1(x_1)\psi_1(x_2)\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$.

A. 1 only B. 2 only C. 3 only D. 2 and 3 only
E. none of the above

Identical Particles

Choose all of the following wavefunctions that are possible for **two identical spin-$^1/_2$ particles** in a one-dimensional infinite square well with width a. The wavefunction for a single particle in a one-dimensional infinite square well is $\psi_n \sim \sin\left(\frac{n\pi x}{a}\right)$ and "A" is a suitable normalization constant.

(1)A $\left[\sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{3\pi x_2}{a}\right) + \sin\left(\frac{3\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right)\right](|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

(2) A $\sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{3\pi x_2}{a}\right)(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

(3) A $\left[\sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{3\pi x_2}{a}\right) - \sin\left(\frac{3\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right)\right]|\uparrow\uparrow\rangle$

A. 3 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only
E. All of the above

Identical Particles

There are two identical **spin-1 particles** in a one dimensional infinite square well. The single particle stationary states are ψ_n (n=1, 2, 3, …). Choose all of the following statements that are correct for the two particle system.

(1) A ground state of the two particle system is $\psi_1(x_1)\psi_1(x_2)(|1,1\rangle\otimes|1,1\rangle)$

(2) $\psi_1(x_1)\psi_2(x_2)(|1,1\rangle\otimes|1,1\rangle)$is one of the first excited state wavefunctions of the two particle system.

(3) A ground state of the two particle system is $\frac{1}{\sqrt{2}}\psi_1(x_1)\psi_1(x_2)(|1,1\rangle\otimes|1,0\rangle + |1,0\rangle\otimes|1,1\rangle)$.

A. 1 and 2 only B. 1 and 3 only C. 2 and 3 only D. all of the above
E. none of the above

Identical Particles

Choose all of the following wavefunctions that are possible for two identical spin-1 particles in a one-dimensional infinite square well with width a. The wavefunction for a single particle in a one-dimensional infinite square well is $\psi_n \sim \sin\left(\frac{n\pi x}{a}\right)$ and "A" is a suitable normalization constant.

(1) $A\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)(|1,1\rangle\otimes|1,1\rangle)$

(2) $A\sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{3\pi x_2}{a}\right)(|1,1\rangle\otimes|1,1\rangle)$

(3) $A\left[\sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{3\pi x_2}{a}\right) - \sin\left(\frac{3\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right)\right](|1,1\rangle\otimes|1,-1\rangle - |1,-1\rangle\otimes|1,1\rangle)$

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only
E. All of the above

Identical Particles

Choose all of the following statements that are true about the Helium atom, a nucleus with two protons orbited by two electrons. (Hint: Consider Coulomb repulsion between electrons.)

1) The ground state of Helium must have an antisymmetric spin configuration with respect to the exchange the electrons (singlet configuration).

2) The energies of the excited states are lower if the electron spins are in the singlet configuration (as opposed to the triplet configuration).

3) The energies of the excited states are lower if the spatial wavefunctions are symmetric with respect to the exchange of the electrons (as opposed to the anti-symmetric configuration).

A. 1 only B. 1 and 3 only C. 2 and 3 only D. All of the above
E. None of the above

Identical Particles

Choose all of the following statements that are correct for a Hydrogen molecule, two spatially separated protons with two electrons orbiting them. (Hint: Consider how the nuclei would come together for bonding to occur.)

(1) The spatial wavefunction is symmetric with respect to the exchange of the electrons in the ground state.

(2) When the spatial wavefunction is symmetric, the electrons have a higher probability of being found between the two protons compared to the case when the spatial wavefunction is anti-symmetric.

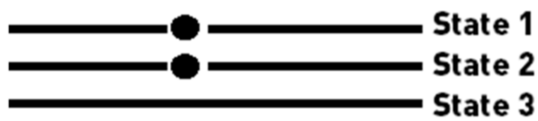
(3) When a covalent bond forms, there is a minimum in the energy and the separation between the two protons is primarily determined by the balance between the electron-proton attraction and proton-proton repulsion.

A. 1 only B. 2 only C. 1 and 3 only D. 2 and 3 only
E. All of the above

B.2 IDENTICAL PARTICLES: COUNTING

Identical Particles

In how many ways can two identical fermions be arranged in a three state system with no constraints on total energy? (One arrangement is shown below)

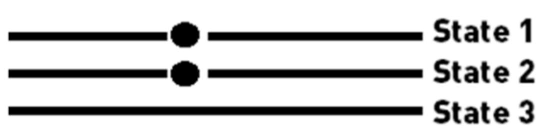


A. $\binom{2}{2} = \frac{2!}{2!\,1!} = 1$ B. $\binom{3}{2} = \frac{3!}{2!\,1!} = 3$ C. $\binom{4}{2} = \frac{4!}{2!\,2!} = 6$

D. $3^2 = 9$ E. $3^3 = 27$

Identical Particles

In how many ways can two identical bosons be arranged in a three state system with no constraints on total energy? (Hint: Consider using the "bin and divider" technique. Here, we have 2 "dividers" between the bins (or states). One arrangement is shown below)



A. $\binom{2}{2} = \frac{2!}{2!\,1!} = 1$ B. $\binom{3}{2} = \frac{3!}{2!\,1!} = 3$ C. $\binom{4}{2} = \frac{4!}{2!\,2!} = 6$

D. $3^2 = 9$ E. $3^3 = 27$

Bosons: Bin & Divider Method

For a system of identical bosons:

- There can be more than one boson in a given single-particle state.
- Treat single-particle states as **bins** to be filled with identical bosons and identical **dividers** to separate the bins.
- Number of distinct many-particle states is the number of ways bosons or dividers can be permuted with each other (permuting two bosons with each other or two dividers with each other does not produce a different state).

Example:

How many ways can two identical bosons be arranged in a three state system?

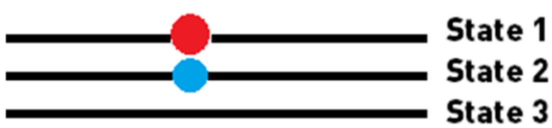
- Since there are three states, it means that there are **two dividers** (number of states – 1) ✖
- There are **two bosons** ●

- There are two bosons that need to be permuted among 4 total objects (two dividers + two bosons) OR two dividers that need to be permuted among 4 total objects (two dividers + two bosons)

$$\binom{Bosons+Dividers}{Bosons} = \binom{4}{2} = \frac{4!}{2!(4-2)!} = 6 \ \underline{\textbf{OR}} \ \binom{Bosons+Dividers}{dividers} = \binom{4}{2} = \frac{4!}{2!(4-2)!} = 6$$

Identical Particles

In how many ways can two distinguishable particles be arranged in a three state system with no constraints on total energy? (One arrangement is shown below)



A. $\binom{2}{2} = \frac{2!}{2!\,1!} = 1$ B. $\binom{3}{2} = \frac{3!}{2!\,1!} = 3$ C. $\binom{4}{2} = \frac{4!}{2!\,2!} = 6$

D. $3^2 = 9$ E. $3^3 = 27$

Class Discussion

For N fermions and n states, the number of possible distinct many-particle states is $\binom{n}{N} = \frac{n!}{N!(n-N)!}$. ($n \geq N$ required)

For N bosons and n states, the number of possible distinct many- particle states is $\binom{n-1+N}{N} = \frac{(n-1+N)!}{N!(n-1)!}$.

For N particles that can be treated as distinguishable and n states, the number of possible distinct many-particle states is n^N.

Why do bosons and distinguishable particles have different numbers of distinct many-particle states?

Identical Particles

Suppose you have three particles and three distinct single-particle states $\psi_a(x), \psi_b(x), \psi_c(x)$. Choose all of the following statements that are correct.

1) If the three particles are distinguishable particles, you can construct 27 different three particle states.
2) If the three particles are identical bosons, you can construct nine different three-particle states.
3) If the three particles are identical fermions, you can construct only one three-particle state.

A. 1 and 2 only B. 1 and 3 only B. 2 and 3 only D. 3 only
E. All of the above

Identical Particles

For one particle in a one dimensional infinite square well ($V(x) = 0$ for $0 \leq x \leq a$) , the energy is $E_n = n^2 K$, where $K = \frac{\pi^2 \hbar^2}{2ma^2}$. What is the number of distinct many-particle states for a three particle system in this 1-D well with total three-particle energy 99K if the particles are fermions, bosons, or distinguishable? Ignore spin.
(Note: 1^2+7^2+7^2 = 5^2+5^2+7^2 = 99)

Answer Choice	Fermion	Boson	Distinguishable
A	1	2	9
B	No possible arrangements	3	9
C	1	3	6
D	No possible arrangements	2	6
E		None of the above	

Identical Particles

For one particle in a one dimensional infinite square well ($V(x) = 0$ for $0 \leq x \leq a$) , the energy is $E_n = n^2 K$, where $K = \frac{\pi^2 \hbar^2}{2ma^2}$. What is the number of distinct many-particle states for a three particle system in this 1-D well with total three-particle energy 243K if the particles are fermions, bosons, or distinguishable? Ignore spin.

(Note: 1^2+11^2+11^2 = 3^2+3^2+15^2= 5^2+7^2+13^2= 9^2+9^2+9^2 = 243)

Answer Choice	Fermion	Boson	Distinguishable
A	1	4	13
B	4	12	24
C	No possible arrangements	4	12
D	1	12	12
E		None of the above	

B.3 DEGENERATE PERTURBATION THEORY

Notes to Students

In perturbation theory, $\widehat{H} = \widehat{H}^0 + \widehat{H}'$ (with the usual definitions)

This results in corrections to the unperturbed energies and wavefunctions as follows:

- $E_n = E_n{}^0 + E_n{}^1 \ldots$
- $\psi_n = \psi_n{}^0 + \psi_n{}^1 \ldots$

In *degenerate* perturbation theory, it is typically necessary to find a "good" basis

What is a "good" basis?

A good basis is one in which the unperturbed Hamiltonian $\widehat{H}^0$ is diagonal and the perturbation Hamiltonian $\widehat{H}'$ is diagonal in each degenerate sub-space of $\widehat{H}^0$.

Here we only focus on 1st order corrections to energies and wavefunctions.

Degenerate Perturbation Theory

For non-degenerate perturbation theory, the first order correction to the nth perturbed energy $E_n{}^1$ is $E_n{}^1 = \langle \psi_n{}^0 | \widehat{H}' | \psi_n{}^0 \rangle$. The first order correction to the nth stationary state $\psi_n{}^1$ can be written as a superposition of the unperturbed wavefunctions $\psi_m{}^0$, $\psi_n{}^1 = \sum_{m \neq n} c_m{}^{(n)} \psi_m{}^0$, where $c_m{}^{(n)} = \frac{\langle \psi_m{}^0 | \widehat{H}' | \psi_n{}^0 \rangle}{E_n{}^0 - E_m{}^0}$ for $m \neq n$. To use the equations for degenerate perturbation theory, it is important to choose a "good" basis.

Choose all of the following statements that are correct about finding a "good" basis.

(1) If there is degeneracy in $\widehat{H}^0$, the denominator of $c_m{}^{(n)} = \frac{\langle \psi_m{}^0 | \widehat{H}' | \psi_n{}^0 \rangle}{E_n{}^0 - E_m{}^0}$ is zero for certain m, n.

(2) A "good" basis is one in which the perturbation Hamiltonian $\widehat{H}'$ is diagonal.

(3) A "good" basis is one in which the perturbation Hamiltonian $\widehat{H}'$ is diagonal in each degenerate sub-space of the unperturbed Hamiltonian $\widehat{H}^0$, such that the numerator of $c_m{}^{(n)} = \frac{\langle \psi_m{}^0 | \widehat{H}' | \psi_n{}^0 \rangle}{E_n{}^0 - E_m{}^0}$ is zero when $E_n{}^0 = E_m{}^0$.

A. 1 only
B. 2 only
C. 3 only
D. 1 and 2 only
E. 1 and 3 only

Degenerate Perturbation Theory

For non-degenerate perturbation theory, the first order correction to the nth perturbed energy ${E_n}^1$ is ${E_n}^1 = \langle {\psi_n}^0 \,|\hat{H}'|{\psi_n}^0 \rangle$. The first order correction to the nth stationary state ${\psi_n}^1$ can be written as a superposition of the unperturbed wavefunctions ${\psi_m}^0$, ${\psi_n}^1 = \sum_{m\neq n} {c_m}^{(n)} {\psi_m}^0$, where ${c_m}^{(n)} = \frac{\langle {\psi_m}^0|\hat{H}'|{\psi_n}^0\rangle}{{E_n}^0 - {E_m}^0}$ for $m \neq n$. To use the equations for degenerate perturbation theory, it is important to choose a "good" basis.

Choose all of the following statements that are correct about finding a "good" basis.

(1) If there is degeneracy in the eigenvalue spectrum of $\hat{H}^0$, one must ensure the basis is a "good" basis for finding the corrections to the wavefunctions ${\psi_n}^1$. Some of the coefficients ${c_m}^{(n)}$ for the corrections to the wavefunctions may "blow up."

(2) If there is degeneracy in the eigenvalue spectrum of $\hat{H}^0$, ***any*** basis that consists of eigenstates of $\hat{H}^0$ can be used to find the corrections to the energies ${E_n}^1$ because ${E_n}^1 = \langle {\psi_n}^0 \,|\hat{H}'|{\psi_n}^0 \rangle$ doesn't have terms that "blow up."

(3) The matrices $\hat{H}^0$ and $\hat{H}'$ need to be represented in the same basis to find perturbative corrections to the energies and wavefunctions.

A. 1 only
B. 1 and 2 only
C. 1 and 3 only
D. 2 and 3 only
E. All of the above

Degenerate Perturbation Theory

Three students are calculating the first order perturbative corrections for a system with unperturbed Hamiltonian $\hat{H}^0$ and perturbation $\hat{H}'$. Because there is a degeneracy in $\hat{H}^0$, they know that they must ensure the basis is a "good" basis in order to use degenerate perturbation theory. Consider the following conversation:

- Student 1: We should not diagonalize the entire $\hat{H}'$ matrix, but rather only the part of $\hat{H}'$ that corresponds to each degenerate subspace of $\hat{H}^0$.
- Student 2: I disagree. If we diagonalize part of the $\hat{H}'$ matrix then we cannot guarantee that it will give us a "good" basis. We must diagonalize the entire $\hat{H}'$ matrix.
- Student 3: Actually, it is equally valid to diagonalize either the entire $\hat{H}'$ matrix or only the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$. We usually choose to diagonalize $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ simply because it requires less work to diagonalize a matrix with a lower dimension.

Which student(s) do you agree with?

A. Student 1 only
B. Student 2 only
C. Student 3 only
D. None of the above

Class Discussion

A "good" basis is one in which the perturbation Hamiltonian $\hat{H}'$ is diagonal in each degenerate sub-space of the unperturbed Hamiltonian $\hat{H}^0$.

The unperturbed Hamiltonian $\hat{H}^0$ is still diagonal in a "good" basis.

Once a "good" basis $\left\{\left|\psi_m{}^0\right\rangle\right\}$ has been found, the first order corrections are:

$$\psi_n{}^1 = \sum_{m\neq n} c_m{}^{(n)}\psi_m{}^0, \text{ where } c_m{}^{(n)} = \frac{\langle\psi_m{}^0|\hat{H}'|\psi_n{}^0\rangle}{E_n{}^0 - E_m{}^0} \text{ for } m \neq n.$$

$$E_n{}^1 = \langle\psi_n{}^0|\hat{H}'|\psi_n{}^0\rangle$$

Degenerate Perturbation Theory

Consider the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}' = V_0\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 2\end{pmatrix} + V_0\begin{pmatrix}-\varepsilon & 0 & 0\\ 0 & 0 & \varepsilon\\ 0 & \varepsilon & 0\end{pmatrix} = V_0\begin{pmatrix}1-\varepsilon & 0 & 0\\ 0 & 1 & \varepsilon\\ 0 & \varepsilon & 2\end{pmatrix}$, where $\varepsilon \ll 1$. The basis vectors for the matrix in the order $|a\rangle$, $|b\rangle$, and $|c\rangle$ are the energy eigenstates of the unperturbed Hamiltonian $\hat{H}^0$ ($\varepsilon = 0$). Choose all of the following statements that are correct about the <u>unperturbed</u> system.

(1) The distinct energies of the unperturbed system are V_0 and $2V_0$.

(2) The $\hat{H}^0$ matrix in the degenerate subspace of $\hat{H}^0$ is $V_0\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$.

(3) The unperturbed Hamiltonian $\hat{H}^0$ has a two-fold degeneracy with energy V_0.

A. 1 only
B. 1 and 2 only
C. 1 and 3 only
D. 2 and 3 only
E. All of the above.

Degenerate Perturbation Theory

Consider the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} + V_0 \begin{pmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{pmatrix} = V_0 \begin{pmatrix} 1-\varepsilon & 0 & 0 \\ 0 & 1 & \varepsilon \\ 0 & \varepsilon & 2 \end{pmatrix}$, where $\varepsilon \ll 1$. The basis vectors for the matrix $|a\rangle$, $|b\rangle$, and $|c\rangle$ (in that order) are the energy eigenstates of the unperturbed Hamiltonian $\hat{H}^0$ ($\varepsilon = 0$). Choose all of the following statements that are correct.

(1) The perturbation matrix in the degenerate subspace of $\hat{H}^0$ is $V_0 \begin{pmatrix} -\varepsilon & 0 \\ 0 & 0 \end{pmatrix}$.
(2) $|a\rangle$ is a "good" state for the perturbation $\hat{H}'$.
(3) $|c\rangle$ is a "good" state for the perturbation $\hat{H}'$.

A. 1 only
B. 1 and 2 only
C. 1 and 3 only
D. 2 and 3 only
E. All of the above

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} + V_0 \begin{pmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{pmatrix} = V_0 \begin{pmatrix} 1-\varepsilon & 0 & 0 \\ 0 & 1 & \varepsilon \\ 0 & \varepsilon & 2 \end{pmatrix}, \text{ where } \varepsilon \ll 1.$$

The degenerate subspace for the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation matrix $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ are highlighted above.

Because the off-diagonal terms of $\hat{H}'$ are zero in the degenerate sub-space of $\hat{H}^0$, the given basis is **already** a "good" basis.

Degenerate Perturbation Theory

Consider the same unperturbed Hamiltonian, $\hat{H}^0$, with a **different perturbation**, $\hat{H}'$.

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} + V_0\begin{pmatrix} -\varepsilon & \varepsilon & 0 \\ \varepsilon & \varepsilon & \varepsilon \\ 0 & \varepsilon & \varepsilon \end{pmatrix} = V_0\begin{pmatrix} 1-\varepsilon & \varepsilon & 0 \\ \varepsilon & 1+\varepsilon & \varepsilon \\ 0 & \varepsilon & 2+\varepsilon \end{pmatrix}, \text{ where } \varepsilon \ll 1.$$

The basis vectors for the matrix $|a\rangle$, $|b\rangle$, and $|c\rangle$ are the energy eigenstates of the unperturbed Hamiltonian $\hat{H}^0$ $(\varepsilon = 0)$. Choose all of the following statements that are correct.

(1) The perturbation matrix in the degenerate subspace of $\hat{H}^0$ is $V_0\begin{pmatrix} -\varepsilon & \varepsilon \\ \varepsilon & \varepsilon \end{pmatrix}$.

(2) $|a\rangle$ is a "good" state for the perturbation $\hat{H}'$.

(3) $|c\rangle$ is a "good" state for the perturbation $\hat{H}'$.

A. 1 only
B. 1 and 2 only
C. 1 and 3 only
D. 2 and 3 only
E. All of the above.

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} + V_0\begin{pmatrix} -\varepsilon & \varepsilon & 0 \\ \varepsilon & \varepsilon & \varepsilon \\ 0 & \varepsilon & \varepsilon \end{pmatrix} = V_0\begin{pmatrix} 1-\varepsilon & \varepsilon & 0 \\ \varepsilon & 1+\varepsilon & \varepsilon \\ 0 & \varepsilon & 2+\varepsilon \end{pmatrix}, \text{ where } \varepsilon \ll 1.$$

The degenerate subspace for the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation matrix $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ are highlighted above.

Because the off-diagonal terms of $\hat{H}'$ are **not** zero in the degenerate sub-space of $\hat{H}^0$, this is **not** a "good" basis.

We need to find a "good" basis because:

1) The corrections to the wavefuntions don't work in this basis as seen here:

$$c_a^{(b)} = \frac{\langle \psi_a{}^0 | \hat{H}' | \psi_b{}^0 \rangle}{E_b{}^0 - E_a{}^0} = \frac{\varepsilon V_0}{2V_0 - 2V_0} = \frac{\varepsilon}{0}, \text{ which diverges.}$$

2) Since the corrections to the wave functions diverge in this basis, $E_n{}^1 = \langle \psi_n{}^0 | \hat{H}' | \psi_n{}^0 \rangle$ will **not** give the right corrections to the energies in this basis.

To find a "good" basis, $\hat{H}'$ must be diagonalized in the degenerate subspace of $\hat{H}^0$. Because $\hat{H}^0$ is effectively an identity matrix in this subspace, it will remain diagonal for any linear combination of those basis vectors.

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} + V_0 \begin{pmatrix} -\varepsilon & \varepsilon & 0 \\ \varepsilon & \varepsilon & \varepsilon \\ 0 & \varepsilon & \varepsilon \end{pmatrix} = V_0 \begin{pmatrix} 1-\varepsilon & \varepsilon & 0 \\ \varepsilon & 1+\varepsilon & \varepsilon \\ 0 & \varepsilon & 2+\varepsilon \end{pmatrix}, \text{ where } \varepsilon \ll 1.$$

To find a "good" basis, we will diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. The basis vectors for the matrix are in the order $|a\rangle$, $|b\rangle$, and $|c\rangle$. We will diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ (the $|a\rangle$, $|b\rangle$ subspace).

Upon diagonalization, $\hat{H}' = \varepsilon V_0 \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}$ becomes $\hat{H}' = \varepsilon V_0 \begin{pmatrix} -\sqrt{2} & 0 \\ 0 & \sqrt{2} \end{pmatrix}$, where the new basis vectors are linear combinations of $|a\rangle$ and $|b\rangle$, in the 2x2 subspace where $\hat{H}^0$ is degenerate, with corrections to the energies $-\sqrt{2}\,\varepsilon V_0$ and $\sqrt{2}\,\varepsilon V_0$ and eigenvectors $\frac{|a\rangle+(1-\sqrt{2})|b\rangle}{\sqrt{4-2\sqrt{2}}}$ and $\frac{|a\rangle+(1+\sqrt{2})|b\rangle}{\sqrt{4+2\sqrt{2}}}$).

In this "good" basis: $\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{pmatrix} 1-\sqrt{2}\varepsilon & 0 & 0 \\ 0 & 1+\sqrt{2}\varepsilon & \varepsilon \\ 0 & \varepsilon & 2+\varepsilon \end{pmatrix} = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} + V_0 \begin{pmatrix} -\sqrt{2}\varepsilon & 0 & 0 \\ 0 & \sqrt{2}\varepsilon & \varepsilon \\ 0 & \varepsilon & \varepsilon \end{pmatrix}$

Therefore, the first order corrections to the energies are $-\sqrt{2}\varepsilon$, $\sqrt{2}\varepsilon$, and ε.

Note that $\hat{H}^0$ remains unchanged in the new basis.

Degenerate Perturbation Theory

Consider the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{pmatrix} 2-\varepsilon & 0 & \varepsilon \\ 0 & 1-\varepsilon & \varepsilon \\ \varepsilon & \varepsilon & 2 \end{pmatrix}$, where $\varepsilon \ll 1$. The basis vectors for the matrix in the order $|a\rangle$, $|b\rangle$, and $|c\rangle$ are the energy eigenstates of the unperturbed Hamiltonian $\hat{H}^0$ ($\varepsilon = 0$). Choose all of the following statements that are correct about the unperturbed system.

(1) The distinct energies of the unperturbed system are V_0 and $2V_0$.
(2) The $\hat{H}^0$ matrix in the degenerate subspace of $\hat{H}^0$ is $V_0 \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}$.
(3) The unperturbed Hamiltonian $\hat{H}^0$ has a two-fold degeneracy with energy $2V_0$.

A. 1 only
B. 1 and 2 only
C. 1 and 3 only
D. 2 and 3 only
E. All of the above.

Degenerate Perturbation Theory

Consider the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}' = V_0\begin{pmatrix} 2-\varepsilon & 0 & \varepsilon \\ 0 & 1-\varepsilon & \varepsilon \\ \varepsilon & \varepsilon & 2 \end{pmatrix}$, where $\varepsilon \ll 1$. The basis vectors for the matrix in the order $|a\rangle$, $|b\rangle$, and $|c\rangle$ are the energy eigenstates of the unperturbed Hamiltonian $\hat{H}^0$ ($\varepsilon = 0$). Choose all of the following statements that are correct.

(1) The perturbation matrix in the degenerate subspace of $\hat{H}^0$ is $V_0\begin{pmatrix} -\varepsilon & 0 \\ 0 & -\varepsilon \end{pmatrix}$.
(2) $|a\rangle$ is a "good" state for the perturbation $\hat{H}'$.
(3) $|c\rangle$ is a "good" state for the perturbation $\hat{H}'$.

A. 1 only
B. 3 only
C. 1 and 2 only
D. 2 and 3 only
E. None of the above.

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0\begin{pmatrix} 2-\varepsilon & 0 & \varepsilon \\ 0 & 1-\varepsilon & \varepsilon \\ \varepsilon & \varepsilon & 2 \end{pmatrix}, \text{ where } \varepsilon \ll 1.$$

The degenerate subspace for the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation matrix $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ are highlighted above.
To see it more clearly, we can stay in the same basis, but reorder the basis vectors: $|a\rangle$, $|c\rangle$, and $|b\rangle$.

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} + V_0\begin{pmatrix} -\varepsilon & \varepsilon & 0 \\ \varepsilon & 0 & \varepsilon \\ 0 & \varepsilon & -\varepsilon \end{pmatrix} = V_0\begin{pmatrix} 2-\varepsilon & \varepsilon & 0 \\ \varepsilon & 2 & \varepsilon \\ 0 & \varepsilon & 1-\varepsilon \end{pmatrix}, \text{ where } \varepsilon \ll 1.$$

Because the off-diagonal terms of $\hat{H}'$ are non-zero in the degenerate sub-space of $\hat{H}^0$, this is **not** a "good" basis.

We need to find a "good" basis because:

1) The corrections to the wavefuntions don't work in this basis as seen here:
$c_a^{(b)} = \frac{\langle \psi_a{}^0 | \hat{H}' | \psi_b{}^0 \rangle}{E_c{}^0 - E_a{}^0} = \frac{\varepsilon V_0}{2V_0 - 2V_0} = \frac{\varepsilon}{0}$, which diverges.

2) Since the corrections to the wave functions diverge in this basis, $E_n{}^1 = \langle \psi_n{}^0 | \hat{H}' | \psi_n{}^0 \rangle$ will **not** give the right corrections to the energies in this basis.

To find a "good" basis, $\hat{H}'$ must be diagonalized in the degenerate subspace of $\hat{H}^0$. Because $\hat{H}^0$ is effectively an identity matrix in this subspace, it will remain diagonal for any linear combination of those basis vectors.

Degenerate Perturbation Theory

Consider the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}' = V_0\begin{pmatrix} 1-\varepsilon & \varepsilon & 0 \\ \varepsilon & 2 & \varepsilon \\ 0 & \varepsilon & 1 \end{pmatrix}$, where $\varepsilon \ll 1$. The basis vectors for the matrix $|a\rangle$, $|b\rangle$, and $|c\rangle$ are the energy eigenstates of the unperturbed Hamiltonian $\hat{H}^0$ ($\varepsilon = 0$). Choose all of the following statements that are correct.

(1)The perturbation matrix in the degenerate subspace of $\hat{H}^0$ is $V_0\begin{pmatrix} -\varepsilon & \varepsilon \\ \varepsilon & 0 \end{pmatrix}$.
(2) $|a\rangle$ is a "good" state for the perturbation $\hat{H}'$.
(3) $|c\rangle$ is a "good" state for the perturbation $\hat{H}'$.

A. 1 only
B. 1 and 2 only
C. 1 and 3 only
D. 2 and 3 only
E. All of the above.

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0\begin{pmatrix} 1-\varepsilon & \varepsilon & 0 \\ \varepsilon & 2 & \varepsilon \\ 0 & \varepsilon & 1 \end{pmatrix} = V_0\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} + V_0\begin{pmatrix} -\varepsilon & \varepsilon & 0 \\ \varepsilon & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{pmatrix}, \text{ where } \varepsilon \ll 1.$$

The degenerate subspace for the unperturbed Hamiltonian $\hat{H}^0$ is highlighted above for both the $\hat{H}^0$ and $\hat{H}'$ matrices.

Because the off-diagonal terms of $\hat{H}'$ are zero in the degenerate sub-space of $\hat{H}^0$, the given basis is **already** a "good" basis.

Class Discussion

In perturbation theory, $\hat{H} = \hat{H}^0 + \hat{H}'$, where $\hat{H}' \ll \hat{H}^0$.

The corrections to the unperturbed energies and wavefunctions are as follows:
$E_n = E_n{}^0 + E_n{}^1 \dots$
$\psi_n = \psi_n{}^0 + \psi_n{}^1 \dots$

In *degenerate* perturbation theory, it is typically necessary to find a "good" basis.

A good basis is one in which both the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation Hamiltonian $\hat{H}'$ are diagonal in the sub-space in which $\hat{H}^0$ has degeneracy.

Next, we will apply degenerate perturbation theory to the Hamiltonian of a Hydrogen atom in an external magnetic field to find the corrections to the energies.

Let's first consider some operators that constitute $\hat{H}^0$ or $\hat{H}'$ in the Hamiltonian for the hydrogen atom:

- $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$ is the unperturbed Hamiltonian that accounts for only the Coulomb interaction of the electron with the nucleus.
- $\hat{H}'_{SO} = \left(\frac{e^2}{8\pi\varepsilon_0}\right)\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}$ is the spin-orbit coupling perturbation term.
- $\hat{H}'_r = \left(\frac{-\hat{p}^4}{8m^3c^2}\right)$ is the relativistic correction to kinetic energy perturbation term.
- $\hat{H}'_{fs} = \hat{H}'_{SO} + \hat{H}'_r$ is the sum of the spin-orbit term and relativistic correction term, called the fine structure perturbation term.

For **all** questions related to the perturbations to the unperturbed Hamiltonian $\hat{H}^0$ of the Hydrogen atom, we will **fix the quantum number *n*** when finding a "good" basis. We do this because we are only concerned with ensuring that $\hat{H}'$ is diagonal in each degenerate subspace of $\hat{H}^0$ to find the corrections to the energies. Since the energy eigenvalues of $\hat{H}^0$ ($2n^2$ degeneracy) are determined by *n*, we need only consider one value of **quantum number *n*** at a time.

Choose all of the following that are correct about the unperturbed Hamiltonian, $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$:

1) The eigenvalues of $\hat{H}^0$ are only dependent on the quantum number n.
2) For a given n, the unperturbed Hamiltonian $\hat{H}^0$ is diagonal in the "coupled" representation, with basis vectors $\left|n, l, s, j, m_j\right\rangle$.
3) For a given n, the unperturbed Hamiltonian $\hat{H}^0$ is diagonal in the "uncoupled" representation, with basis vectors $\left|n, l, m_l, s, m_s\right\rangle$.

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only E. All of the above

Class Discussion

In both the coupled and uncoupled representations, $\hat{H}^0$ is diagonal. Below is the matrix for either representation, with <u>*n*=2</u>.

Because $\hat{H}^0$ is spherically symmetric, any arbitrary orthonormal angular basis found with a linear combination of a complete set of the coupled or uncoupled states with the same quantum number n is a "good" angular basis.

On the right is a table showing the basis vectors we will be using for each representation.

In this case, the unperturbed Hamiltonian $\hat{H}^0$ is 8-fold degenerate for n=2. For simplicity, we will define $E_2 = -\frac{13.6eV}{4}$.

$$\hat{H}^0 = E_2\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Now let's take a look at the relativistic correction term and the spin-orbit coupling term, which together make up the fine structure perturbation, $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$.

	l	**Uncoupled** $\left|m_l, m_s\right\rangle$	**Coupled** $\left|j, m_j\right\rangle$
$\left|\psi_1\right\rangle$	$l = 0$	$\left|0, \frac{1}{2}\right\rangle$	$\left|\frac{1}{2}, \frac{1}{2}\right\rangle$
$\left|\psi_2\right\rangle$		$\left|0, \frac{-1}{2}\right\rangle$	$\left|\frac{1}{2}, \frac{-1}{2}\right\rangle$
$\left|\psi_3\right\rangle$	$l = 1$	$\left|1, \frac{1}{2}\right\rangle$	$\left|\frac{3}{2}, \frac{3}{2}\right\rangle$
$\left|\psi_4\right\rangle$		$\left|1, \frac{-1}{2}\right\rangle$	$\left|\frac{3}{2}, \frac{-3}{2}\right\rangle$
$\left|\psi_5\right\rangle$		$\left|0, \frac{1}{2}\right\rangle$	$\left|\frac{3}{2}, \frac{1}{2}\right\rangle$
$\left|\psi_6\right\rangle$		$\left|0, \frac{-1}{2}\right\rangle$	$\left|\frac{1}{2}, \frac{1}{2}\right\rangle$
$\left|\psi_7\right\rangle$		$\left|-1, \frac{1}{2}\right\rangle$	$\left|\frac{3}{2}, \frac{-1}{2}\right\rangle$
$\left|\psi_8\right\rangle$		$\left|-1, \frac{-1}{2}\right\rangle$	$\left|\frac{1}{2}, \frac{-1}{2}\right\rangle$
Note: for all vectors above, $n = 2, s = \frac{1}{2}$			

For a fixed n, choose all of the following that are correct about the relativistic correction term, $\hat{H}'_r = \left(\frac{-\hat{p}^4}{8m^3c^2}\right)$:

1) Since $\hat{H}'_r$ is spherically symmetric and the corresponding relativistic correction to the energy depends on quantum numbers n and l, any arbitrary orthonormal basis found with a linear combination of a complete set of the coupled or uncoupled states with the same quantum numbers n and l is a "good" angular basis for this perturbation.
2) The coupled representation, with basis vectors $\left|n, l, s, j, m_j\right\rangle$, is a basis in which both $\hat{H}'_r$ and $\hat{H}^0$ is diagonal and $\hat{H}'_r$ is diagonal in each degenerate subspace of $\hat{H}^0$.
3) The uncoupled representation, with basis vectors $|n, l, m_l, s, m_s\rangle$, is a basis in which both $\hat{H}'_r$ and $\hat{H}^0$ is diagonal and $\hat{H}'_r$ is diagonal in each degenerate subspace of $\hat{H}^0$.

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only E. All of the above

For fixed n, $\hat{H}^0$ is diagonal and $\hat{H}'_r$ is diagonal in each degenerate subspace of $\hat{H}^0$ in both the uncoupled and coupled representation. Choose all of the following that are correct about the relativistic correction term, $\hat{H}'_r = \left(\frac{-\hat{p}^4}{8m^3c^2}\right)$:

1) The coupled representation is a "good" angular basis for $\hat{H}'_r$.
2) The uncoupled representation is a "good" angular basis for $\hat{H}'_r$.
3) Any arbitrary complete orthonormal basis found with linear combinations of a complete set of the coupled or uncoupled states with the same quantum number l is a "good" angular basis for this perturbation.

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only E. All of the above

Choose all of the following that are correct about the spin-orbit coupling term,

$$\hat{H}'_{SO} = \left(\frac{e^2}{8\pi\varepsilon_0}\right)\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}$$

(Hint: $\vec{S}\cdot\vec{L} = \frac{1}{2}\left(\hat{J}^2 - \hat{L}^2 - \hat{S}^2\right) = \frac{1}{2}\left(\hat{S}_+\,\hat{L}_- + \hat{S}_-\,\hat{L}_+\right) + \hat{S}_Z\,\hat{L}_Z$):

1) The spin-orbit coupling term, $\hat{H}'_{SO}$, is spherically symmetric, just like the unperturbed Hamiltonian, $\hat{H}^0$, and the relativistic correction term, $\hat{H}'_r$.
2) In each degenerate subspace of $\hat{H}^0$, the spin-orbit term is diagonal in the coupled representation, with basis vectors $\left|n, l, s, j, m_j\right\rangle$.
3) In each degenerate subspace of $\hat{H}^0$, the spin-orbit term is diagonal in the uncoupled representation, with basis vectors $\left|n, l, m_l, s, m_s\right\rangle$.

A. 1 only B. 2 only C. 3 only D. 1 and 2 only E. None of the above

So far we have learned that, in each degenerate subspace of $\hat{H}^0$:

$\hat{H}^0$ is diagonal in both the coupled and uncoupled representations.
$\hat{H}'_{SO}$ is diagonal in the coupled representation, but not in the uncoupled representation.

Choose all of the following that are correct about the spin-orbit coupling term,
$\hat{H}'_{SO} = \left(\frac{e^2}{8\pi\varepsilon_0}\right)\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}$:

1) The coupled representation is a "good" angular basis for $\hat{H}'_{SO}$.
2) The uncoupled representation is a "good" angular basis for $\hat{H}'_{SO}$.
3) Any arbitrary complete orthonormal basis found with linear combinations of a complete set of the coupled states is a "good" angular basis for $\hat{H}'_{SO}$.

A. 1 only B. 2 only C. 3 only D. 1 and 3 only E. None of the above

So far we have learned that, in each degenerate subspace of $\hat{H}^0$:

$\hat{H}^0$ is diagonal in both the coupled and uncoupled representations.
$\hat{H}'_r$ is diagonal in both the coupled and uncoupled representations.
$\hat{H}'_{SO}$ is diagonal in the coupled representation, but not in the uncoupled representation.

Choose all of the following that are correct about the fine structure term,

$$\hat{H}'_{fs} = \hat{H}'_{SO} + \hat{H}'_r = \left(\frac{e^2}{8\pi\varepsilon_0}\right)\frac{1}{m^2c^2r^3}\hat{\vec{S}}\cdot\hat{\vec{L}} - \left(\frac{\hat{p}^4}{8m^3c^2}\right)$$

(Hint: $\hat{\vec{S}}\cdot\hat{\vec{L}} = \frac{1}{2}\left(\hat{J}^2 - \hat{L}^2 - \hat{S}^2\right) = \frac{1}{2}\left(\hat{S}_+\hat{L}_- + \hat{S}_-\hat{L}_+\right) + \hat{S}_Z\hat{L}_Z$):

1) The coupled representation is a "good" angular basis for $\hat{H}'_{fs}$.
2) The uncoupled representation is a "good" angular basis for $\hat{H}'_{fs}$.
3) Any arbitrary complete orthonormal basis found with linear combinations of the coupled states is a "good" angular basis for this perturbation.

A. 1 only B. 2 only C. 3 only D. 1 and 3 only E. None of the above

Class Discussion

Hamiltonian	Uncoupled Representation	Coupled Representation
$\hat{H}^0$	Diagonal	Diagonal
$\hat{H}'_r$	Diagonal	Diagonal
$\hat{H}'_{SO}$	Not Diagonal	Diagonal
$\hat{H}'_{fs}$	Not Diagonal	Diagonal

The fine-structure correction to the Hamiltonian is $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$.

In each degenerate subspace of $\hat{H}^0$, the relativistic correction term is diagonal in both the coupled and uncoupled representations.

In each degenerate subspace of $\hat{H}^0$, the spin-orbit coupling term is diagonal only in the coupled representation.

Therefore, the coupled representation is a "good" angular basis for determining the perturbative corrections to energies and wavefunctions for the fine-structure perturbation.

Now we will consider perturbations due to the Zeeman effect when the atom is placed in an external magnetic field in the $\hat{z}$ direction.

Choose all of the following that are correct about the Zeeman term due to an external magnetic field in the $\hat{z}$ direction, $\hat{H}'_Z = \frac{e}{2m}(\vec{L} + 2\vec{S}) \cdot \vec{B}_{ext} = \mu_B B_{ext}(\hat{L}_Z + 2\hat{S}_Z) = \mu_B B_{ext}(\hat{J}_Z + \hat{S}_Z)$:

1) In each degenerate subspace of $\hat{H}^0$, the Zeeman term is diagonal in the uncoupled representation, with basis vectors $|n, l, m_l, s, m_s\rangle$ because $\hat{L}_Z$ and $\hat{S}_Z$ are diagonal in that basis.
2) In each degenerate subspace of $\hat{H}^0$, the Zeeman term is diagonal in the coupled representation, with basis vectors $|n, l, s, j, m_j\rangle$ because $\hat{J}_Z$ is diagonal in that basis.
3) In each degenerate subspace of $\hat{H}^0$, the Zeeman term is **not** diagonal in the coupled representation, with basis vectors $|n, l, s, j, m_j\rangle$ because $\hat{S}_Z$ is **not** diagonal in that basis.

A. 1 only B. 2 only C. 1 and 2 only D. 1 and 3 only E. None of the above

Choose all of the following that are correct about the Zeeman term due to an external magnetic field in the $\hat{z}$ direction, $\hat{H}'_Z = \frac{e}{2m}(\vec{L} + 2\vec{S}) \cdot \vec{B}_{ext} = \mu_B B_{ext}(\hat{L}_Z + 2\hat{S}_Z) = \mu_B B_{ext}(\hat{J}_Z + \hat{S}_Z)$:

1) The Zeeman term is diagonal in the uncoupled representation, with basis vectors $|n, l, m_l, s, m_s\rangle$.
2) The Zeeman term is diagonal in the coupled representation, with basis vectors $|n, l, s, j, m_j\rangle$.
3) If there were no fine structure correction to take into account, the Zeeman effect would not involve perturbation theory since we can find simultaneous eigenstates of both $\hat{H}^0$ and $\hat{H}'_Z$ (the entire $\hat{H}^0$ and the Zeeman term can be diagonalized simultaneously).

A. 1 only B. 2 only C. 1 and 2 only D. 1 and 3 only E. None of the above

Class Discussion

For a fixed n (in the degenerate subspace of $\widehat{H}^0$), the fine-structure correction to the Hamiltonian is only diagonal in the coupled representation.

The Zeeman term is only diagonal in the uncoupled representation.

Hamiltonian	Uncoupled Representation	Coupled Representation
$\widehat{H}^0$	Diagonal	Diagonal
$\widehat{H}'_r$	Diagonal	Diagonal
$\widehat{H}'_{so}$	Not Diagonal	Diagonal
$\widehat{H}'_{fs}$	Not Diagonal	Diagonal
$\widehat{H}'_Z$	Diagonal	Not Diagonal

Next, we will discuss how to find the corrections to the energies for systems with both Zeeman and fine-structure perturbations.

Note: When considering the Zeeman effect, the fine-structure term must always be included since it is **not** negligible.

For a hydrogen atom with fixed quantum number n, the Zeeman term in the perturbation is given by $\widehat{H}'_Z = \mu_B B_{ext}(\hat{L}_Z + 2\hat{S}_Z) = \mu_B B_{ext}(\hat{J}_Z + \hat{S}_Z)$. Choose all of the following statements that are true about the intermediate field Zeeman effect, for which neither the Zeeman term $\widehat{H}'_Z$ nor the fine structure term $\widehat{H}'_{fs}$ dominates ($\widehat{H}'_Z \sim \widehat{H}'_{fs}$).

1) The "good" angular basis states for the perturbation are the coupled states $|n, l, s, j, m_j\rangle$.
2) The "good" angular basis states for the perturbation are the uncoupled states $|n, l, m_l, s, m_s\rangle$.
3) Both the coupled and uncoupled states are "good" angular states for the perturbation.

A. 1 only B. 2 only C. 3 only D. Not enough information E. None of the above

In the case of an intermediate field Zeeman effect, for which neither the Zeeman term $\hat{H}'_Z$ nor the fine structure term $\hat{H}'_{fs}$ dominates $(\hat{H}'_Z \sim \hat{H}'_{fs})$, neither the coupled nor uncoupled representation is a "good" angular basis. Choose all of the following that are correct about finding the perturbative corrections to energies and wavefunctions with the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$:

1) To find the perturbative corrections to energies and wavefunctions, either the coupled or uncoupled representations can be chosen as the initial basis, and then $\hat{H}'$ must be diagonalized in each degenerate subspace of $\hat{H}^0$.
2) The corrections to the energies will depend on the initial choice of basis before finding a "good" angular basis by diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.
3) Regardless of whether you choose the coupled or uncoupled representation as your initial basis, once you diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$, you'll end up with the same first order perturbative corrections to the energies.

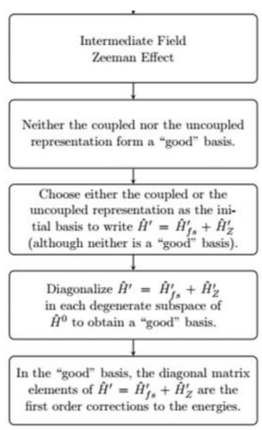
A. 1 only B. 2 only C. 3 only D. 1 and 2 only E. 1 and 3 only

In order to find the first order corrections to the energies for the intermediate field Zeeman effect, we can start in either the coupled or uncoupled representation and diagonalize $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$.

The perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ is shown below in the coupled representation for n=2. Basis vectors are shown on the right, in the order chosen to construct the matrix, for reference. $\gamma = \frac{-13.6eV\,\alpha^2}{64}$, $\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c}$, and $\beta = \mu_B B_{ext}$.

$$\hat{H}' = \begin{bmatrix} 5\gamma-\beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5\gamma+\beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma-2\beta & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma+2\beta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \left[\begin{matrix} \gamma-\frac{2}{3}\beta \\ \frac{\sqrt{2}}{3}\beta \end{matrix}\right. & \left.\begin{matrix} \frac{\sqrt{2}}{3}\beta \\ 5\gamma-\frac{1}{3}\beta \end{matrix}\right] & 0 & 0 \\ 0 & 0 & 0 & 0 & & & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \left[\begin{matrix} \gamma+\frac{2}{3}\beta \\ \frac{\sqrt{2}}{3}\beta \end{matrix}\right. & \left.\begin{matrix} \frac{\sqrt{2}}{3}\beta \\ 5\gamma+\frac{1}{3}\beta \end{matrix}\right] \\ 0 & 0 & 0 & 0 & 0 & 0 & & \end{bmatrix}$$

Because $\hat{H}^0$ is 8-fold degenerate for $n = 2$, the two bracketed 2x2 subspaces in the perturbation above must be diagonalized in order to find a "good" angular basis and determine the first order perturbative corrections to the energies.



	l	**Coupled** $\left\|j, m_j\right\rangle$
$\|\psi_1\rangle$	$l = 0$	$\left\|\frac{1}{2}, \frac{1}{2}\right\rangle$
$\|\psi_2\rangle$		$\left\|\frac{1}{2}, \frac{-1}{2}\right\rangle$
$\|\psi_3\rangle$	$l = 1$	$\left\|\frac{3}{2}, \frac{3}{2}\right\rangle$
$\|\psi_4\rangle$		$\left\|\frac{3}{2}, \frac{-3}{2}\right\rangle$
$\|\psi_5\rangle$		$\left\|\frac{3}{2}, \frac{1}{2}\right\rangle$
$\|\psi_6\rangle$		$\left\|\frac{1}{2}, \frac{1}{2}\right\rangle$
$\|\psi_7\rangle$		$\left\|\frac{3}{2}, \frac{-1}{2}\right\rangle$
$\|\psi_8\rangle$		$\left\|\frac{1}{2}, \frac{-1}{2}\right\rangle$
Note: for all vectors above, $n = 2, s = \frac{1}{2}$		

The Zeeman term in the perturbation can be **strong** ($\hat{H}'_Z \gg \hat{H}'_{fs}$) or **weak** ($\hat{H}'_Z \ll \hat{H}'_{fs}$) relative to the fine structure term.

In the following slides:

1. First, we will consider the **strong** field Zeeman ($\hat{H}'_Z \gg \hat{H}'_{fs}$).
2. Then, we will consider the **weak** field Zeeman ($\hat{H}'_Z \ll \hat{H}'_{fs}$).

We will see how we can handle these perturbations differently in these extreme cases.

For a fixed *n,* choose all of the following statements that are true about the **strong** field Zeeman effect, $\hat{H}'_Z \gg \hat{H}'_{fs}$. We can use a two-step process in which we first take into account $\hat{H}'_Z$ as the stronger perturbation and then take the weaker perturbation $\hat{H}'_{fs}$ into account in the second step.

1) In the first step of the two-step approximation, $\hat{H}'_Z$ is diagonal when the uncoupled representation is chosen as the basis so it is diagonal in the degenerate subspace of $\hat{H}^0$.
2) In the second step of the two-step approximation, the new Hamiltonian $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ is diagonal and the perturbation $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}_Z^0$ in the uncoupled representation.
3) The uncoupled representation will never be a "good" angular basis in the second step of the two-step approximation because $\hat{H}'_{fs}$ is **not** diagonal in the degenerate subspace of $\hat{H}^0$ in the uncoupled representation.

A. 1 only B. 2 only C.3 only D. 1 and 2 only E. 1 and 3 only

For the **strong** field Zeeman effect, $\hat{H}'_Z \gg \hat{H}'_{fs}$, we can first take into account $\hat{H}'_Z$ as the stronger perturbation, and then take the weaker $\hat{H}'_{fs}$ into account as a second perturbation.

Taking $\hat{H}'_Z$ as the perturbation in **step 1**, we must diagonalize $\hat{H}'_Z$ in the degenerate subspace of $\hat{H}^0$. Then in **step 2**, we must treat $\hat{H}'_{fs}$ as the perturbation on $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$.

Because the **uncoupled** representation is already a "good" angular basis for $\hat{H}'_Z$, we can use that as the initial basis. Basis vectors are shown on the right , in the order chosen to construct the matrix, for reference.

$$\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z = -\frac{13.6\text{eV}}{4}\begin{bmatrix} 1&0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0\\ 0&0&0&1&0&0&0&0\\ 0&0&0&0&1&0&0&0\\ 0&0&0&0&0&1&0&0\\ 0&0&0&0&0&0&1&0\\ 0&0&0&0&0&0&0&1 \end{bmatrix} + \mu_B B_{ext}\begin{bmatrix} 1&0&0&0&0&0&0&0\\ 0&-1&0&0&0&0&0&0\\ 0&0&2&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&0&1&0&0&0\\ 0&0&0&0&0&-1&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&-2 \end{bmatrix}$$

	l	**Uncoupled** $\lvert m_l, m_s\rangle$
$\lvert\psi_1\rangle$	$l=0$	$\lvert 0,\frac{1}{2}\rangle$
$\lvert\psi_2\rangle$		$\lvert 0,\frac{-1}{2}\rangle$
$\lvert\psi_3\rangle$	$l=1$	$\lvert 1,\frac{1}{2}\rangle$
$\lvert\psi_4\rangle$		$\lvert 1,\frac{-1}{2}\rangle$
$\lvert\psi_5\rangle$		$\lvert 0,\frac{1}{2}\rangle$
$\lvert\psi_6\rangle$		$\lvert 0,\frac{-1}{2}\rangle$
$\lvert\psi_7\rangle$		$\lvert -1,\frac{1}{2}\rangle$
$\lvert\psi_8\rangle$		$\lvert -1,\frac{-1}{2}\rangle$
Note: for all vectors above, $n=2, s=\frac{1}{2}$		

For a **strong** field Zeeman effect, $\hat{H}'_Z \gg \hat{H}'_{fs}$, we can first take into account $\hat{H}'_Z$ as the stronger perturbation, and then take the weaker $\hat{H}'_{fs}$ into account as a second perturbation.

Take $\hat{H}'_Z$ as the perturbation and choose the uncoupled representation in **step 1**. In **step 2**, treat $\hat{H}'_{fs}$ as the perturbation on $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$. Here, we see that some of the 8-fold degeneracy of $\hat{H}^0$ has been broken by including the Zeeman term as the perturbation in **step 1**. Now, we have three separate degenerate 2x2 subspaces for $\hat{H}^0_Z$ remaining.

$$\hat{H}^0_Z = \begin{bmatrix} \boxed{E_2+\mu_B B_{ext}}&0&0&0&0&0&0&0\\ 0&\underline{E_2-\mu_B B_{ext}}&0&0&0&0&0&0\\ 0&0&E_2+2\mu_B B_{ext}&0&0&0&0&0\\ 0&0&0&E_2&0&0&0&0\\ 0&0&0&0&\boxed{E_2+\mu_B B_{ext}}&0&0&0\\ 0&0&0&0&0&\underline{E_2-\mu_B B_{ext}}&0&0\\ 0&0&0&0&0&0&E_2&0\\ 0&0&0&0&0&0&0&E_2-2\mu_B B_{ext} \end{bmatrix}$$

For convenience, we can reorder our basis vectors as shown in the right column of the table.

$$\hat{H}^0_Z = \begin{bmatrix} E_2+\mu_B B_{ext}&0&0&0&0&0&0&0\\ 0&E_2+\mu_B B_{ext}&0&0&0&0&0&0\\ 0&0&E_2-\mu_B B_{ext}&0&0&0&0&0\\ 0&0&0&E_2-\mu_B B_{ext}&0&0&0&0\\ 0&0&0&0&E_2&0&0&0\\ 0&0&0&0&0&E_2&0&0\\ 0&0&0&0&0&0&E_2+2\mu_B B_{ext}&0\\ 0&0&0&0&0&0&0&E_2-2\mu_B B_{ext} \end{bmatrix}$$

	Uncoupled (1st) $\lvert l,m_l,m_s\rangle$	**Uncoupled (2nd)** $\lvert l,m_l,m_s\rangle$
$\lvert\psi_1\rangle$	$\lvert 0,0,\frac{1}{2}\rangle$	$\lvert 0,0,\frac{1}{2}\rangle$
$\lvert\psi_2\rangle$	$\lvert 0,0,\frac{-1}{2}\rangle$	$\lvert 1,0,\frac{1}{2}\rangle$
$\lvert\psi_3\rangle$	$\lvert 1,1,\frac{1}{2}\rangle$	$\lvert 0,0,\frac{-1}{2}\rangle$
$\lvert\psi_4\rangle$	$\lvert 1,1,\frac{-1}{2}\rangle$	$\lvert 1,0,\frac{-1}{2}\rangle$
$\lvert\psi_5\rangle$	$\lvert 1,0,\frac{1}{2}\rangle$	$\lvert 1,1,\frac{-1}{2}\rangle$
$\lvert\psi_6\rangle$	$\lvert 1,0,\frac{-1}{2}\rangle$	$\lvert 1,-1,\frac{1}{2}\rangle$
$\lvert\psi_7\rangle$	$\lvert 1,-1,\frac{1}{2}\rangle$	$\lvert 1,1,\frac{1}{2}\rangle$
$\lvert\psi_8\rangle$	$\lvert 1,-1,\frac{-1}{2}\rangle$	$\lvert 1,-1,\frac{-1}{2}\rangle$
Note: for all vectors above, $n=2, s=\frac{1}{2}$		

Finally, for a **strong** field Zeeman effect, $\hat{H}'_Z \gg \hat{H}'_{fs}$, in **step** 2, the weaker perturbation $\hat{H}'_{fs}$ can be treated as a perturbation on $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$. In uncoupled representation with basis vectors listed in the table to the right, we can see both $\hat{H}_Z^0$ and perturbation $\hat{H}'_{fs}$ for n=2.

$$\hat{H}_Z^0 = \begin{bmatrix} E_2+\mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_2+\mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_2-\mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_2-\mu_B B_{ext} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_2+2\mu_B B_{ext} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_2-2\mu_B B_{ext} \end{bmatrix}$$

Even though the perturbation $\hat{H}'_{fs}$ has off-diagonal terms in this basis, it is diagonal in the degenerate subspaces of $\hat{H}_Z^0$ and the uncoupled representation is a "good" angular basis with the diagonal elements of $\hat{H}'_{fs}$ giving the first order corrections to the energies.

$$\hat{H}'_{fs} = \frac{(-13.6\text{ eV})\alpha^2}{192} \begin{bmatrix} 15 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 7 & 0 & 0 & 4\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 15 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 7 & 0 & 4\sqrt{2} & 0 & 0 \\ 0 & 4\sqrt{2} & 0 & 0 & 11 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4\sqrt{2} & 0 & 11 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix}$$

	Uncoupled $\lvert l, m_l, m_s\rangle$
$\lvert\psi_1\rangle$	$\lvert 0,0,\frac{1}{2}\rangle$
$\lvert\psi_2\rangle$	$\lvert 1,0,\frac{1}{2}\rangle$
$\lvert\psi_3\rangle$	$\lvert 0,0,\frac{-1}{2}\rangle$
$\lvert\psi_4\rangle$	$\lvert 1,0,\frac{-1}{2}\rangle$
$\lvert\psi_5\rangle$	$\lvert 1,1,\frac{-1}{2}\rangle$
$\lvert\psi_6\rangle$	$\lvert 1,-1,\frac{1}{2}\rangle$
$\lvert\psi_7\rangle$	$\lvert 1,1,\frac{1}{2}\rangle$
$\lvert\psi_8\rangle$	$\lvert 1,-1,\frac{-1}{2}\rangle$
Note: for all vectors above, $n=2, s=\frac{1}{2}$	

Now let's consider the **weak** field Zeeman effect, $\hat{H}'_Z \ll \hat{H}'_{fs}$. Choose all of the following statements that are true about the **weak** field Zeeman effect, $\hat{H}'_Z \ll \hat{H}'_{fs}$. We can use a two-step process in which we first take into account $\hat{H}'_{fs}$ as the stronger perturbation and then take the weaker perturbation $\hat{H}'_Z$ into account in the second step.

1) In the first step of the two-step approximation, $\hat{H}'_{fs}$ is diagonal in the degenerate subspace of $\hat{H}^0$ when the coupled representation is chosen as the basis.
2) In the second step of the two-step approximation, the new Hamiltonian $\hat{H}_{fs}^0 = \hat{H}^0 + \hat{H}'_{fs}$ is diagonal and the perturbation $\hat{H}'_Z$ is diagonal in each degenerate subspace of $\hat{H}_{fs}^0$ in the coupled representation.
3) The coupled representation will never be a "good" angular basis in the second step of the two-step approximation because $\hat{H}'_Z$ is **not** diagonal in the degenerate subspace of $\hat{H}^0$ in the coupled representation.

A. 1 only B. 2 only C.3 only D. 1 and 2 only E. 1 and 3 only

For a **<u>weak</u>** field Zeeman effect, $\hat{H}'_{fs} \gg \hat{H}'_Z$, we can first take into account $\hat{H}'_{fs}$ as the stronger perturbation and then take the weaker perturbation $\hat{H}'_Z$ into account as a second perturbation.

Taking $\hat{H}'_{fs}$ as the perturbation in **step 1**, we must diagonalize $\hat{H}'_{fs}$ in the degenerate subspace of $\hat{H}^0$. Then in **step 2,** we must treat $\hat{H}'_Z$ as the perturbation on $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$.

Because the **coupled** representation is already a "good" angular basis for $\hat{H}'_{fs}$, we can choose that as the initial basis. Basis vectors are shown on the right, in the order chosen to construct the matrix, for reference for *n*=2.
(Note: $E_2 = \frac{-13.6eV}{4}$)

$$\hat{H}^0_{fs} = \begin{bmatrix} E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} \end{bmatrix}$$

We can see that the 8-fold degeneracy of $\hat{H}^0$ has been broken into two 4x4 degenerate subspaces by $\hat{H}'_{fs}$.

	l	Coupled $\lvert j, m_j\rangle$
$\lvert\psi_1\rangle$	$l = 1$	$\lvert\frac{3}{2}, \frac{3}{2}\rangle$
$\lvert\psi_2\rangle$		$\lvert\frac{3}{2}, \frac{1}{2}\rangle$
$\lvert\psi_3\rangle$		$\lvert\frac{3}{2}, \frac{-1}{2}\rangle$
$\lvert\psi_4\rangle$		$\lvert\frac{3}{2}, \frac{-3}{2}\rangle$
$\lvert\psi_5\rangle$		$\lvert\frac{1}{2}, \frac{1}{2}\rangle$
$\lvert\psi_6\rangle$		$\lvert\frac{1}{2}, \frac{-1}{2}\rangle$
$\lvert\psi_7\rangle$	$l = 0$	$\lvert\frac{1}{2}, \frac{1}{2}\rangle$
$\lvert\psi_8\rangle$		$\lvert\frac{1}{2}, \frac{-1}{2}\rangle$
Note: for all vectors above, $n = 2, s = \frac{1}{2}$		

For the **<u>weak</u>** field Zeeman effect, $\hat{H}'_{fs} \gg \hat{H}'_Z$, in **step 2** the weaker perturbation $\hat{H}'_Z$ can be treated as a perturbation on $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$. In the coupled representation with basis vectors listed in the table to the right, in the order chosen to construct the matrix, $\hat{H}^0_{fs}$ and perturbation $\hat{H}'_Z$ are shown below for *n*=2:

$$\hat{H}^0_{fs} = \begin{bmatrix} E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} \end{bmatrix}$$

$$\hat{H}'_Z = \mu_B B_{ext} \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{2}{3} & 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2}{3} & 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & -\frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

Even though the perturbation $\hat{H}'_Z$ has off-diagonal terms in this basis, it is diagonal in the degenerate subspaces of $\hat{H}^0_{fs}$, and the coupled representation is a "good" angular basis with the diagonal elements giving the $\hat{H}'_Z$ corrections to the energies.

	Uncoupled $\lvert l, m_l, m_s\rangle$
$\lvert\psi_1\rangle$	$\lvert 0, 0, \frac{1}{2}\rangle$
$\lvert\psi_2\rangle$	$\lvert 1, 0, \frac{1}{2}\rangle$
$\lvert\psi_3\rangle$	$\lvert 0, 0, \frac{-1}{2}\rangle$
$\lvert\psi_4\rangle$	$\lvert 1, 0, \frac{-1}{2}\rangle$
$\lvert\psi_5\rangle$	$\lvert 1, 1, \frac{-1}{2}\rangle$
$\lvert\psi_6\rangle$	$\lvert 1, -1, \frac{1}{2}\rangle$
$\lvert\psi_7\rangle$	$\lvert 1, 1, \frac{1}{2}\rangle$
$\lvert\psi_8\rangle$	$\lvert 1, -1, \frac{-1}{2}\rangle$
Note: for all vectors above, $n = 2, s = 1/2$	

Class Discussion

Intermediate field Zeeman effect in which neither the Zeeman term nor the fine structure term dominates:

- Choose either coupled representation or uncoupled representation as the initial basis to write $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_{z}$, despite neither being a "good" angular basis for this perturbation.
- Diagonalize $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_{z}$ in the degenerate subspace of $\hat{H}^0$ to find a "good" angular basis.
- The diagonal elements of $\hat{H}'$ in this "good" angular basis are the perturbative corrections to the energies.

Only one perturbative term dominates (strong or weak field Zeeman effect):

- **Step 1:** Treat the dominant perturbation as the perturbation $\hat{H}'_{strong}$ on $\hat{H}^0$.
  - If $\hat{H}'_{strong} = \hat{H}'_{Z}$, the uncoupled representation is a "good" angular basis. (Strong Field Zeeman Effect)
  - If $\hat{H}'_{strong} = \hat{H}'_{fs}$, the coupled representation is a "good" angular basis. (Weak Field Zeeman Effect)
- **Step 2:** Consider perturbation $\hat{H}'_{weak}$ on $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$.
  - For special cases $\hat{H}'_{fs} \gg \hat{H}'_{Z}$ and $\hat{H}'_{fs} \ll \hat{H}'_{Z}$, degeneracies of $\hat{H}^0$ are broken in $\hat{H}^0_{strong}$ such that the basis in **step 1** is still "good" angular for $\hat{H}'_{weak}$ in **step 2**.

Degenerate Perturbation Theory

For an unperturbed Hamiltonian $\hat{H}^0$, suppose we know the explicit form of the nth stationary state wavefunction ${\psi_n}^0$. If the perturbation Hamiltonian $\hat{H}'$ is given explicitly, choose all of the following statements that are correct.

(1) The first order correction to the nth energy ${E_n}^1$, depends on the other unperturbed wavefunctions ${\psi_m}^0$ $(m = 1,2,3 \dots, n-1, n+1 \dots)$

(2) The expression for the first order correction to the wavefunction ${\psi_n}^1$ involves knowledge of the first order correction to the energy ${E_n}^1$.

(3) If there is a degeneracy in the unperturbed Hamiltonian, a "good" basis must be chosen in order to determine the corrections to the stationary state wave functions and energies.

A. 1 only
B. 2 only
C. 3 only
D. 2 and 3 only
E. none of the above

Degenerate Perturbation Theory

Suppose eigenstates $|a\rangle$, $|b\rangle$, and $|c\rangle$ of a 3-dimensional $\widehat{H}^0$ are 2-fold degenerate and a perturbation $\widehat{H}'$ acts on this system. Choose all of the following statements that are correct if $|a\rangle$, $|b\rangle$, and $|c\rangle$ form a "good" basis for the perturbed system. (Define $\langle i|\widehat{H}'|j\rangle = H'_{ij}$).

(1) $H'_{aa} = H'_{bb} = H'_{cc}$
(2) $H'_{ab} = H'_{bc} = H'_{ca} = 0$
(3) $|a\rangle$, $|b\rangle$, and $|c\rangle$ are orthogonal to each other.

A. 1 only
B. 2 only
C. 1 and 3 only
D. 2 and 3 only
E. All of the above

Degenerate Perturbation Theory

In a 3D Hilbert space, $\widehat{H}^0$ is the unperturbed Hamiltonian. $|a\rangle$ and $|b\rangle$ are the 2-fold degenerate energy eigenstates of $\widehat{H}^0$ with energy E_1 and $|c\rangle$ is the energy eigenstate with energy E_2. If $|a\rangle$ and $|b\rangle$ are **not** "good" states for the perturbation $\widehat{H}'$, choose all of the following statements that must be correct.

1) $\mathrm{H}'_{ac} = \mathrm{H}'_{bc} \neq 0$, where $\langle \mathrm{i}|\widehat{\mathrm{H}}'|\mathrm{j}\rangle = \mathrm{H}'_{ij}$.
2) $\mathrm{H}'_{ab} = (\mathrm{H}'_{ab})^* \neq 0$
3) If $\widehat{\mathrm{H}}'$ does not commute with $\widehat{\mathrm{H}}^0$, we can never simultaneously diagonalize both $\widehat{\mathrm{H}}^0$ and $\widehat{\mathrm{H}}'$, meaning we cannot find an exact solution.

A. 2 only
B. 3 only
C. 1 and 2 only
D. 2 and 3 only
E. All of the above

Degenerate Perturbation Theory

Suppose $\hat{H}^0$ and $\hat{H}'$ commute with each other. Choose all of the following statements that are correct.

1) If $\hat{H}^0$ is diagonal in a given basis and there is no degeneracy in the eigenvalue spectrum of $\hat{H}^0$ and $\hat{H}'$, then $\hat{H}'$must be diagonal in that basis.
2) If $\hat{H}^0$ is diagonal in a given basis and there is a degeneracy in the eigenvalue spectrum of $\hat{H}^0$, then $\hat{H}'$must be diagonal in that basis.
3) We can always find a special basis in which both $\hat{H}^0$ and $\hat{H}'$ are diagonal simultaneously.

A. 1 only
B. 1 and 2 only
C. 1 and 3 only
D. 2 and 3 only
E. All of the above